

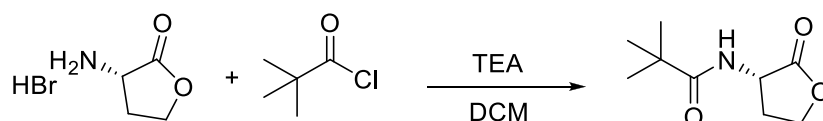
A Key $n \rightarrow \pi^*$ Interaction in *N*-Acyl Homoserine Lactones

Robert W. Newberry[†] and Ronald T. Raines*

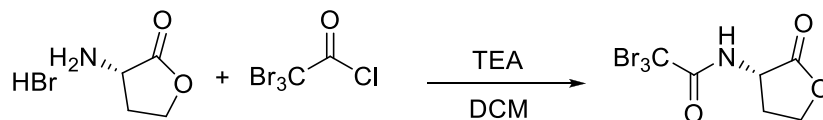
Page	Contents
S1	Table of Contents
S2	Experimental Procedures
S3	Computational Procedures
S4	Figure S1. ¹ H and ¹³ C NMR spectra of <i>N</i> -trimethylacetyl homoserine lactone (1) in CDCl ₃
S5	Figure S2. ¹ H and ¹³ C NMR spectra of <i>N</i> -tribromoacetyl homoserine lactone (2) in CDCl ₃ /H ₂ O
S6	Table S1. Crystal data and structure refinement for 1
S7	Table S2. Atomic coordinates and equivalent isotropic displacement parameters for 1
S7	Table S3. Anisotropic displacement parameters for 1
S8	Table S4. Bond lengths for 1
S8	Table S5. Bond angles for 1
S9	Table S6. Hydrogen coordinates and isotropic displacement parameters for 1
S10	Table S7. Crystal data and structure refinement for 2
S11	Table S8. Atomic coordinates and equivalent isotropic displacement parameters for 2
S11	Table S9. Anisotropic displacement parameters for 2
S12	Table S10. Bond lengths for 2
S12	Table S11. Bond angles for 2
S12	Table S12. Hydrogen coordinates and isotropic displacement parameters for 2
S13	Table S13. Cartesian coordinates of the optimized geometry of 1
S14	Table S14. Cartesian coordinates of the optimized geometry of 2

General Experimental. Commercial chemicals were of reagent grade or better, and were used without further purification. All chemicals were obtained from Sigma–Aldrich (St. Louis, MO). Anhydrous CH_2Cl_2 was obtained from CYCLE-TAINER[®] solvent delivery systems (J. T. Baker, Phillipsburg, NJ). Reactions were monitored by thin-layer chromatography with visualization by UV light or staining with KMnO_4 . Flash chromatography was performed with columns of silica gel 60, 230–400 mesh (Silicycle, Québec City, Canada). The removal of solvents and other volatile materials “under reduced pressure” refers to the use of a rotary evaporator at water-aspirator pressure (<20 torr) and a water bath of <45 °C.

Instrumentation. NMR spectra were acquired at ambient temperature with a Bruker DMX 400 MHz spectrometer (^1H , 400 MHz; ^{13}C , 100 MHz) in the National Magnetic Resonance Facility at Madison (NMRFAM). ^{13}C spectra were proton-decoupled. Mass spectrometry was performed with a Micromass LCT (electrospray ionization, ESI) instrument in the Mass Spectrometry Facility of the Department of Chemistry at the University of Wisconsin–Madison. X-Ray diffraction data were collected in the Molecular Structure Laboratory of the Department of Chemistry at the University of Wisconsin–Madison on a Bruker Quazar SMART APEXII diffractometer.



Synthesis of *N*-trimethylacetyl homoserine lactone (1). (*S*)-(-)- α -Amino- γ -butyrolactone hydrobromide (0.10 g, 0.55 mmol) was dissolved in 10 mL of anhydrous DCM with TEA (0.15 mL, 1.1 mmol). Trimethylacetyl chloride (0.65 mL, 0.55 mmol) was added dropwise, and the resulting mixture was stirred at room temperature overnight. The mixture was then extracted with aqueous hydrochloric acid, followed by saturated aqueous sodium bicarbonate. The organic portion was then dried over anhydrous sodium sulfate, and solvent was removed under reduced pressure. Purification was achieved using silica gel chromatography with 4% v/v methanol in DCM. ^1H NMR (CDCl_3) δ 6.21 (s, 1H), 4.47 (m, 2H), 4.28 (m, 1H), 2.84 (m, 1H), 2.11 (m, 1H), 1.22 (s, 9H); ^{13}C NMR δ 179.1, 175.6, 66.0, 49.3, 38.6, 30.5, 27.4; ESI–MS: $[\text{M} + \text{H}]^+$ calculated 186.1125, found 186.1131.



Synthesis of *N*-tribromoacetyl homoserine lactone (2). (*S*)-(-)- α -Amino- γ -butyrolactone hydrobromide (0.50 g, 2.8 mmol) was dissolved in 20 mL of anhydrous DCM containing TEA (1.15 mL, 8.25 mmol). Tribromoacetyl chloride (0.53 mL, 2.75 mmol) was added dropwise, and the resulting mixture was stirred at room temperature overnight. The mixture was then extracted with aqueous hydrochloric acid, followed by saturated aqueous sodium bicarbonate. The organic portion was then dried over anhydrous sodium sulfate, and solvent was removed under reduced pressure. Purification was achieved using silica gel chromatography with 4% v/v methanol in DCM. ^1H NMR (CDCl_3) δ 7.35 (s, 1H), 4.55 (m, 2H), 4.36 (m, 1H), 2.98 (m, 1H), 2.27 (m, 1H);

^{13}C NMR δ 174.1, 163.1, 66.4, 51.2, 33.9, 29.8; ESI-MS: $[\text{M} + \text{NH}_4]^+$ calculated 394.8237, found 394.8229.

Structure determination by X-ray diffraction analysis. Compounds were dissolved in hexane with a minimal amount of DCM. Slow evaporation afforded diffraction quality crystals in approximately three days. Crystals were selected under oil under ambient conditions and attached to the tip of a MiTeGen MicroMount. The crystal was mounted in a stream of cold nitrogen at 100(1) K and centered in the X-ray beam by using a video camera. Crystal evaluation and data collection were performed on a Bruker SMART APEXII diffractometer with Cu K_α ($\lambda = 1.54178 \text{ \AA}$) radiation for **1** and Mo K_α ($\lambda = 0.71073 \text{ \AA}$) for **2**. Data were collected by using the full-sphere data collection routine to a resolution of 0.80 \AA . The intensity data was then corrected for Lorentz and polarization effects. Absorption was corrected analytically. Structure solution by direct methods was carried out using SHELXTL V.6.10.^{S1} Refinement was performed using the olex2.refine refinement package using Gauss-Newton minimization.^{S2} All non-hydrogen atoms were refined anisotropically. The final difference Fourier maps were featureless.

Computational methodology. Preferred conformations were determined by optimizing the respective compounds at the B3LYP/6-311+G(2d,p) level of theory as implemented by Gaussian 09.^{S3} Frequency calculations of optimized structures yielded no imaginary frequencies, indicating a true minimum on the potential energy surface. Energies were corrected by the zero-point vibrational energy. Optimized geometries were subjected to analysis by NBO 5.9 at the B3LYP/6-311+G(2d,p) level of theory implemented in Gaussian 09.^{S4}

References

- (S1) Sheldrick, G. M. *Acta Cryst.* **2008**, *A64*, 112-122.
- (S2) Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. J. *Appl. Cryst.* **2009**, *42*, 339-341.
- (S3) Gaussian 09, Revision **A.1**, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.
- (S4) NBO 5.9. Glendening, E. D.; Badenhoop, J. k.; Reed, A. E.; Carpenter, J. E.; Bohmann, J. A.; Morales, C. M.; Weinhold, F. Theoretical Chemistry Institute, University of Wisconsin-Madison, Madison, WI, 2012.

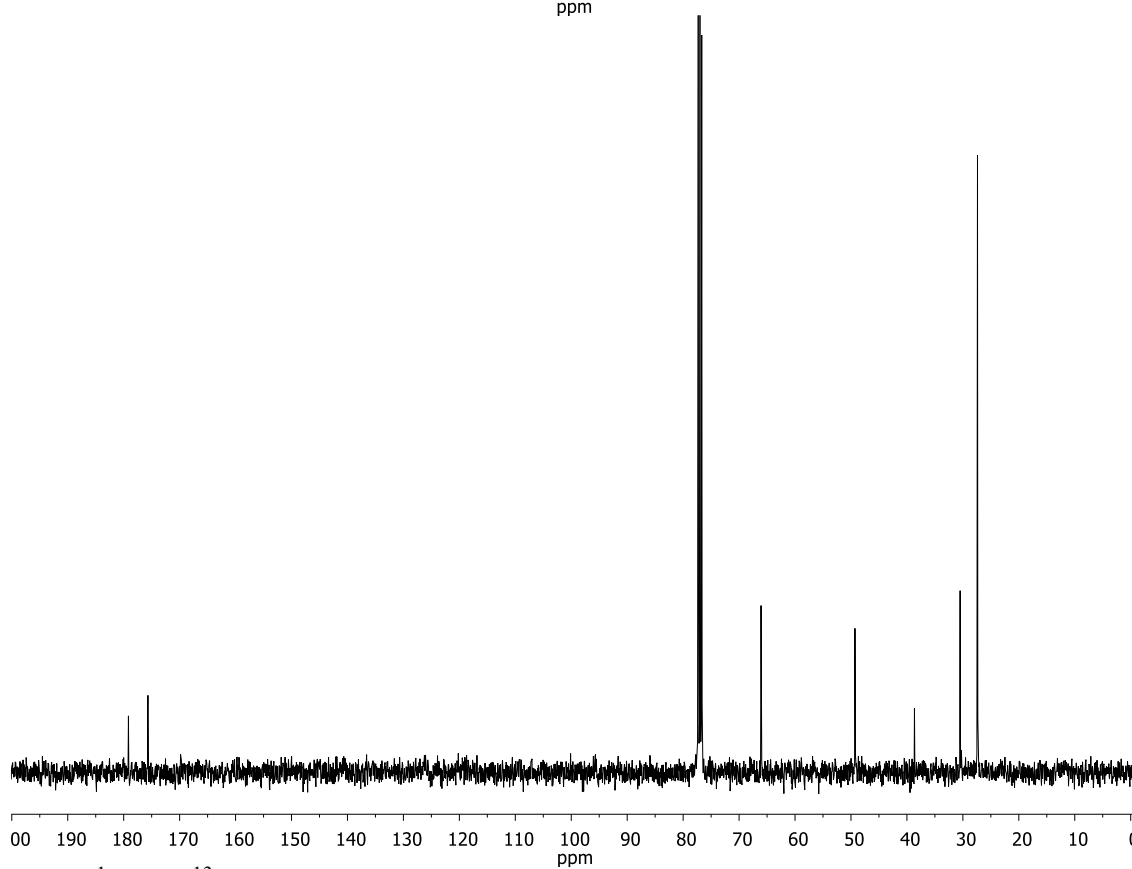
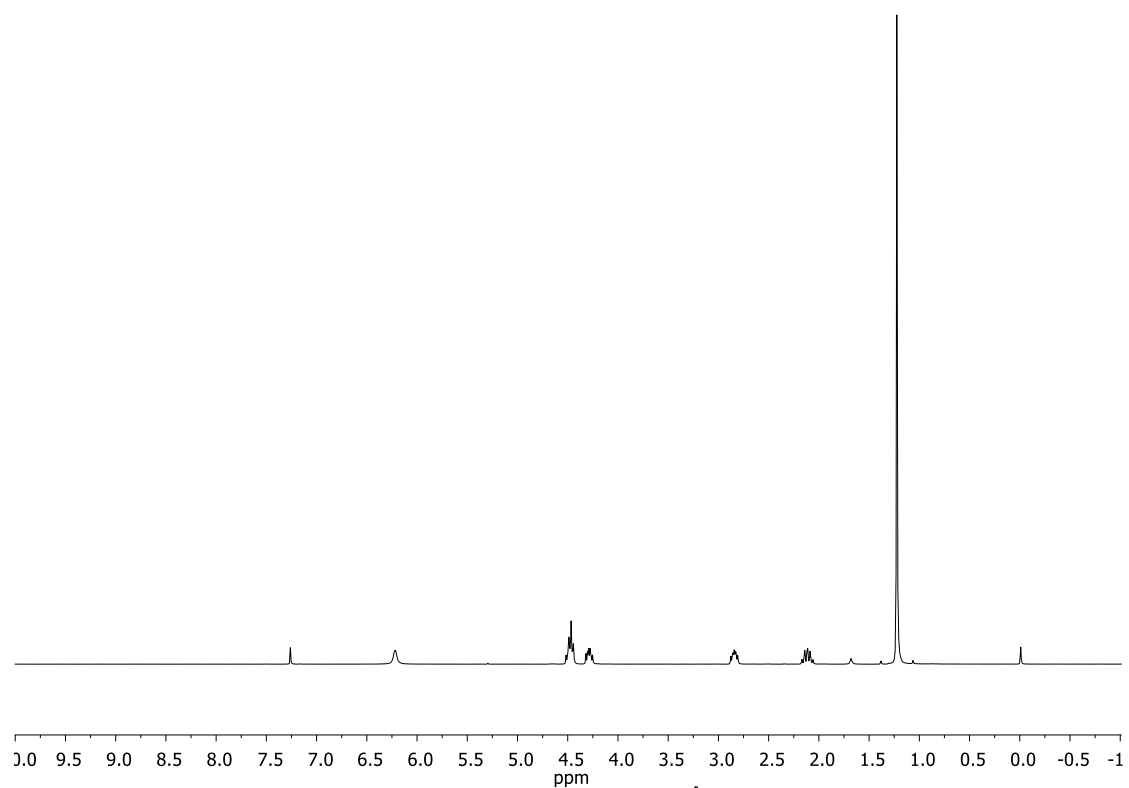


Figure S1. ^1H and ^{13}C NMR spectra of *N*-trimethylacetyl homoserine lactone (**1**) in CDCl_3 .

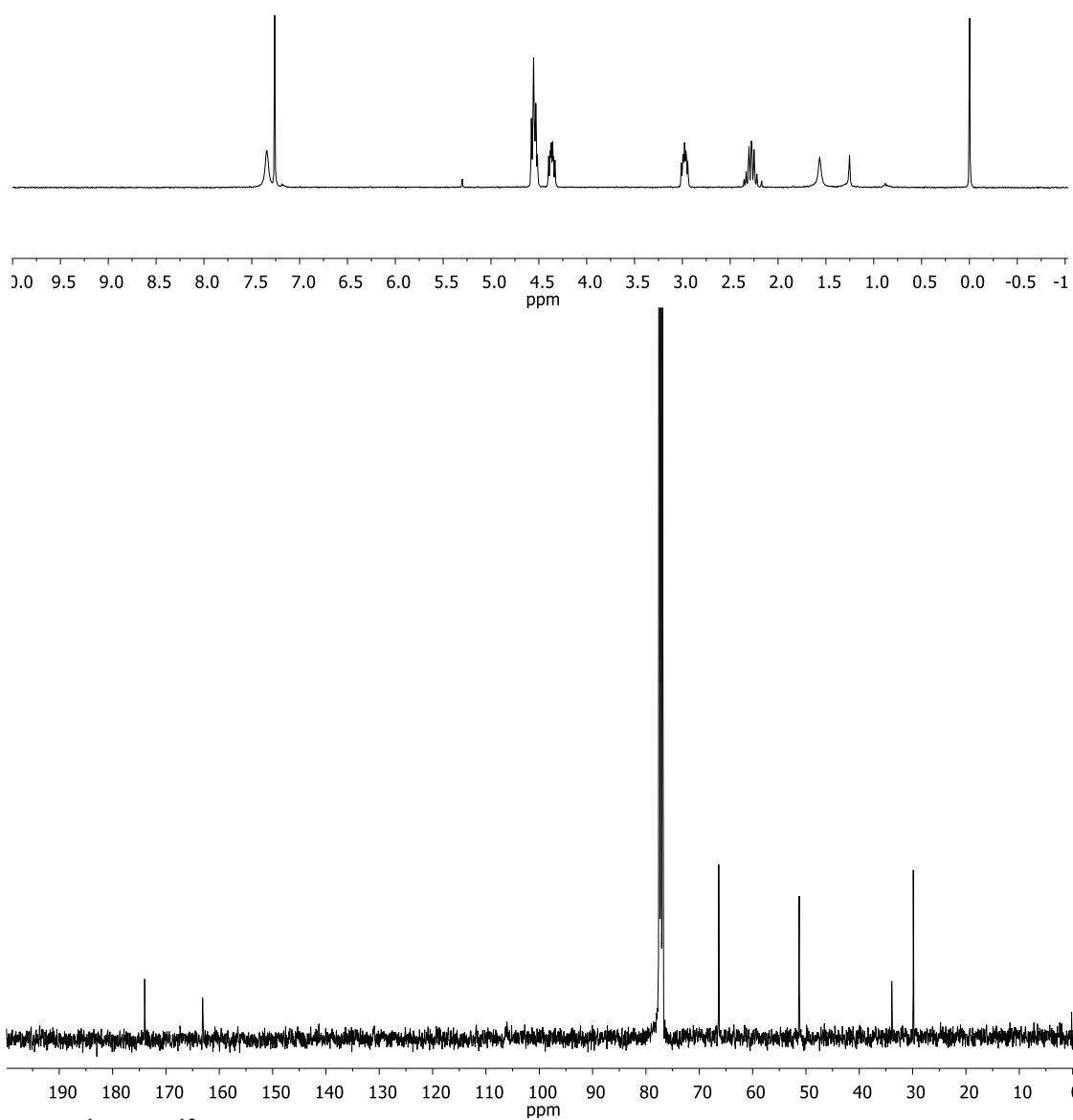


Figure S2. ¹H and ¹³C NMR spectra of *N*-tribromoacetyl homoserine lactone (**2**) in CDCl₃/H₂O.

Table S1. Crystal data and structure refinement for **1**.

Identification code	raines66
Empirical formula	C ₉ H ₁₀ NO ₃
Formula weight	185.22
Temperature/K	100.01
Crystal system	monoclinic
Space group	P2 ₁
<i>a</i> /Å	5.9595(4)
<i>b</i> /Å	9.2235(10)
<i>c</i> /Å	9.2066(6)
α /°	90
β /°	102.719(4)
γ /°	90
Volume/Å ³	493.65(7)
<i>Z</i>	2
ρ_{calc} (mg/mm ³)	1.2460
m/mm ⁻¹	0.771
<i>F</i> ₀₀₀	200.7
Crystal size/mm ³	1.942 × 0.371 × 0.348
2 θ range for data collection	9.84 to 145.38°
Index ranges	-7 ≤ <i>h</i> ≤ 7, -8 ≤ <i>k</i> ≤ 10, -11 ≤ <i>l</i> ≤ 11
Reflections collected	10374
Independent reflections	1721 [<i>R</i> _{int} = 0.0277]
Data/restraints/parameters	1721/0/120
Goodness-of-fit on <i>F</i> ²	1.613
Final <i>R</i> indexes [<i>I</i> ≥ 2 σ _{<i>I</i>}]	<i>R</i> ₁ = 0.0583
Final <i>R</i> indexes [all data]	<i>R</i> ₁ = 0.0584, w <i>R</i> ₂ = 0.1605
Largest diff. peak/hole / e Å ⁻³	0.35/-0.67
Flack parameter	-0.0(2)

Table S2. Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1**. U_{eq} is defined as $1/3$ of the trace of the orthogonalized U_{IJ} tensor.

Atom	x	y	z	U_{eq}
O1	1617(2)	5131.8(17)	8378.8(15)	22.9(4)
O2	4374(2)	4238.6(17)	11934.2(14)	19.6(4)
O3	679(2)	4873.8(17)	11438.7(15)	20.9(4)
N1	243(3)	2940(2)	8815.7(16)	17.2(4)
C1	2178(3)	4079(2)	11210.1(18)	14.5(4)
C6	-1304(3)	4122(2)	6399(2)	17.8(4)
C4	5810(3)	3099(3)	11505(2)	22.5(5)
C2	1936(3)	2756(2)	10196.3(19)	16.4(4)
C5	319(3)	4115(2)	7953(2)	16.2(4)
C3	4404(3)	2486(2)	10051(2)	24.2(5)
C7	-2932(4)	2842(3)	6089(2)	32.0(6)
C8	239(5)	4154(5)	5288(2)	58.8(12)
C9	-2765(7)	5496(4)	6285(4)	70.4(15)

Table S3. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka \times b \times U_{12}]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O1	26.0(7)	20.1(9)	19.9(6)	-8.5(6)	-0.6(5)	0.5(6)
O2	16.1(6)	19.3(8)	21.5(6)	0.2(5)	-0.2(5)	-3.6(6)
O3	18.6(6)	20.0(9)	24.9(7)	2.0(6)	6.6(5)	-1.5(6)
N1	17.2(7)	15.4(9)	16.5(7)	-2.7(6)	-1.7(6)	0.9(6)
C1	14.9(8)	11.7(11)	16.1(8)	-2.8(7)	1.9(6)	1.9(7)
C6	18.3(8)	16.1(10)	17.1(8)	1.4(8)	-0.1(7)	0.8(7)
C4	17.5(8)	28.1(13)	20.5(9)	4.0(8)	1.5(7)	-3.0(8)
C2	16.9(8)	15.1(11)	15.4(8)	0.6(7)	-0.3(6)	1.0(7)
C5	13.4(7)	16.8(11)	17.1(8)	1.0(7)	0.7(6)	-0.2(7)
C3	23.3(9)	27.2(13)	19.9(9)	12.8(9)	0.2(7)	-5.8(9)
C7	32.3(9)	38.4(15)	19.8(9)	-16.5(11)	-6.3(7)	4.6(9)
C8	37.9(12)	121(4)	17.6(10)	-37.3(19)	6.9(9)	-5.7(15)
C9	88(2)	34.8(19)	58(2)	35.2(19)	-50.1(19)	-21.9(15)

Table S4. Bond lengths for **1**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C5	1.224(3)	C6	C5	1.541(2)
O2	C1	1.340(2)	C6	C7	1.515(3)
O2	C4	1.464(3)	C6	C8	1.518(3)
O3	C1	1.209(2)	C6	C9	1.528(3)
N1	C2	1.448(2)	C4	C3	1.523(3)
N1	C5	1.350(3)	C2	C3	1.526(2)
C1	C2	1.524(3)			

Table S5. Bond angles for **1**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C4	O2	C1	110.61(15)	C9	C6	C8	111.0(3)
C5	N1	C2	120.19(16)	C3	C4	O2	105.21(14)
O3	C1	O2	121.68(17)	C1	C2	N1	113.43(16)
C2	C1	O2	110.06(15)	C3	C2	N1	116.16(14)
C2	C1	O3	128.17(15)	C3	C2	C1	102.78(15)
C7	C6	C5	114.62(17)	N1	C5	O1	121.84(16)
C8	C6	C5	106.04(15)	C6	C5	O1	121.16(18)
C8	C6	C7	110.2(2)	C6	C5	N1	117.01(17)
C9	C6	C5	107.40(16)	C2	C3	C4	102.55(15)
C9	C6	C7	107.6(2)				

Table S6. Hydrogen atom coordinates ($\text{\AA} \times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1**.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{eq}
H1	-838(3)	2284(2)	8538.1(16)	20.6(5)
H4a	7282(3)	3505(3)	11358(2)	26.9(6)
H4b	6146(3)	2336(3)	12278(2)	26.9(6)
H2	1450(3)	1918(2)	10743.6(19)	19.7(5)
H3a	4739(3)	3003(2)	9181(2)	29.0(6)
H3b	4704(3)	1438(2)	9959(2)	29.0(6)
H7a	-2052(5)	1939(3)	6290(20)	48.0(8)
H7b	-4040(20)	2898(12)	6733(17)	48.0(8)
H7c	-3760(30)	2861(13)	5044(7)	48.0(8)
H8a	1280(50)	4980(20)	5500(30)	88.2(18)
H8c	1140(50)	3256(19)	5370(30)	88.2(18)
H8b	-709(6)	4240(40)	4277(4)	88.2(18)
H9a	-3510(50)	5544(19)	7130(20)	106(2)
H9b	-1780(12)	6348(4)	6290(40)	106(2)
H9c	-3940(40)	5477(17)	5356(18)	106(2)

Table S7. Crystal data and structure refinement for **2**.

Identification code	Raines67
Empirical formula	C ₆ H ₆ NO ₃ Br ₃
Formula weight	379.83
Temperature/K	100.01
Crystal system	orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁
<i>a</i> /Å	9.559(4)
<i>b</i> /Å	9.933(4)
<i>c</i> /Å	10.094(4)
α /°	90
β /°	90
γ /°	90
Volume/Å ³	958.4(6)
<i>Z</i>	4
ρ_{calc} (mg/mm ³)	2.6321
m/mm ⁻¹	12.598
<i>F</i> ₀₀₀	709.4
Crystal size/mm ³	0.463 × 0.37 × 0.048
Radiation	MoK α (λ = 0.71073)
2 θ range for data collection	5.76 to 61.04°
Index ranges	-13 ≤ <i>h</i> ≤ 13, -14 ≤ <i>k</i> ≤ 14, -14 ≤ <i>l</i> ≤ 14
Reflections collected	22866
Independent reflections	2931 [<i>R</i> _{int} = 0.0611]
Data/restraints/parameters	2931/0/117
Goodness-of-fit on <i>F</i> ²	0.602
Final <i>R</i> indexes [<i>I</i> ≥ 2 σ ₁]	<i>R</i> ₁ = 0.0229
Final <i>R</i> indexes [all data]	<i>R</i> ₁ = 0.0280, <i>wR</i> ₂ = 0.0494
Largest diff. peak/hole / e Å ⁻³	1.44/-0.78
Flack parameter	0.033(15)

Table S8. Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **2**. U_{eq} is defined as $1/3$ of the trace of the orthogonalized U_{IJ} tensor.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U_{eq}
Br1	-583.9(3)	-967.5(3)	-3272.6(4)	11.56(7)
Br2	-2246.3(4)	-1198.7(4)	-5951.1(4)	13.19(7)
Br3	-3792.9(3)	-1710.5(3)	-3241.8(4)	12.12(7)
O1	-1277(3)	-3972(2)	-3136(2)	11.7(4)
O2	-3692(3)	-5885(3)	-3465(3)	19.3(6)
N1	-2065(3)	-4169(3)	-5233(3)	10.3(5)
O3	-2004(3)	-7403(3)	-3748(3)	15.5(5)
C3	-1975(4)	-5613(3)	-5262(3)	9.8(6)
C5	-514(4)	-6238(3)	-5248(4)	11.4(6)
C1	-2039(4)	-1947(3)	-4195(3)	8.4(6)
C2	-1731(3)	-3466(3)	-4154(4)	8.5(6)
C4	-794(4)	-7602(3)	-4606(4)	14.1(7)
C6	-2679(4)	-6267(4)	-4052(4)	13.3(6)

Table S9. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+\dots+2hka\times b\times U_{12}]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Br1	11.58(14)	9.94(14)	13.15(16)	-1.59(11)	-2.62(14)	0.08(13)
Br2	19.54(17)	11.21(14)	8.82(15)	2.69(13)	-1.42(13)	2.63(13)
Br3	9.75(14)	13.06(14)	13.54(16)	2.52(12)	1.67(14)	1.22(14)
O1	15.5(11)	11.7(10)	8.0(11)	1.3(10)	-3.8(10)	-0.9(10)
O2	15.6(12)	22.4(13)	19.9(15)	-3.6(11)	7.2(12)	-0.7(11)
N1	15.4(14)	7.1(12)	8.4(13)	-1.1(10)	-2.3(11)	0.6(10)
O3	18.6(14)	14.3(12)	13.7(13)	-1.8(10)	3.2(10)	3.6(10)
C3	13.5(15)	7.8(13)	8.2(15)	-3.3(12)	-1.4(13)	-0.1(12)
C5	13.1(14)	8.6(13)	12.6(16)	0.3(13)	3.8(13)	0.7(12)
C1	11.5(14)	8.8(13)	4.9(14)	1.0(11)	-0.6(11)	0.3(11)
C2	8.0(13)	5.6(13)	11.8(16)	1.8(11)	1.4(12)	2.6(12)
C4	18.0(17)	8.4(14)	15.8(18)	-0.1(13)	2.9(14)	1.5(13)
C6	10.9(14)	15.3(14)	13.7(15)	-5.2(12)	-3.5(14)	2.2(14)

Table S10. Bond lengths for **2**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br1	C1	1.936(3)	O3	C4	1.458(5)
Br2	C1	1.932(3)	O3	C6	1.336(4)
Br3	C1	1.947(3)	C3	C5	1.528(5)
O1	C2	1.223(4)	C3	C6	1.539(5)
O2	C6	1.197(5)	C5	C4	1.526(5)
N1	C3	1.438(4)	C1	C2	1.538(4)
N1	C2	1.332(5)			

Table S11. Bond angles for **2**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	N1	C3	121.6(3)	C2	C1	Br2	115.0(2)
C6	O3	C4	111.2(3)	C2	C1	Br3	105.7(2)
C5	C3	N1	117.4(3)	N1	C2	O1	123.8(3)
C6	C3	N1	112.3(3)	C1	C2	O1	119.6(3)
C6	C3	C5	102.8(3)	C1	C2	N1	116.5(3)
C4	C5	C3	101.8(3)	C5	C4	O3	105.7(3)
Br2	C1	Br1	108.75(16)	O3	C6	O2	123.0(3)
Br3	C1	Br1	108.65(16)	C3	C6	O2	127.8(3)
Br3	C1	Br2	108.57(16)	C3	C6	O3	109.1(3)
C2	C1	Br1	110.0(2)				

Table S12. Hydrogen atom coordinates ($\text{Å} \times 10^4$) and isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for **2**.

Atom	x	y	z	U(eq)
H1	-2348(3)	-3738(3)	-5946(3)	12.3(7)
H3	-2469(4)	-5936(3)	-6075(3)	11.8(7)
H5a	-138(4)	-6341(3)	-6156(4)	13.7(7)
H5b	146(4)	-5694(3)	-4714(4)	13.7(7)
H4a	26(4)	-7899(3)	-4083(4)	16.9(8)
H4b	-997(4)	-8290(3)	-5289(4)	16.9(8)

Table S13. Cartesian coordinates of the optimized geometry of **1**. SCF Energy = -632.406154 Hartree.

C	2.79423600	-1.14882200	-0.51359800
O	2.89150600	0.27287300	-0.76694000
C	1.38142100	0.06156300	1.04915900
C	2.03953700	-1.30904900	0.81607500
H	2.24967500	-1.58991700	-1.34622100
H	3.81187600	-1.53417600	-0.48382100
H	1.68747100	0.48143200	2.00746500
H	2.73176200	-1.53321900	1.62871700
H	1.30495200	-2.10911800	0.76306200
C	2.00200000	0.96798100	-0.03554900
O	1.78333200	2.13550500	-0.18948300
N	-0.07116000	0.10099100	1.03970900
H	-0.52222200	0.63291800	1.76403000
C	-0.78126300	-0.22349000	-0.07885300
O	-0.21585200	-0.69179800	-1.05756100
C	-2.30827900	-0.01345200	-0.06037200
C	-2.95621700	-1.40087900	-0.23860700
H	-2.73763100	-2.05383400	0.61066900
H	-4.04152100	-1.29843500	-0.31446500
H	-2.58701000	-1.88136400	-1.14444200
C	-2.65291700	0.88029300	-1.26815400
H	-3.73635000	1.00262000	-1.34199000
H	-2.20395000	1.87147900	-1.16873400
H	-2.28624500	0.43373100	-2.19181300
C	-2.83248300	0.63873200	1.22864600
H	-3.91684400	0.75165400	1.16524300
H	-2.62602800	0.02983400	2.11325800
H	-2.41791100	1.63955600	1.38046500

Table S14. Cartesian coordinates of the optimized geometry of **2**. SCF Energy = 8235.128938 Hartree

C	-4.07961800	1.20396900	-0.52940700
O	-4.24591900	-0.21388400	-0.76574000
C	-2.70239000	-0.05585800	1.02546300
C	-3.29298900	1.34297800	0.78496000
H	-3.53505000	1.61339600	-1.37831300
H	-5.07746000	1.63584500	-0.48342600
H	-3.00122700	-0.44928700	1.99634900
H	-3.95736400	1.60992200	1.60709300
H	-2.52166400	2.10658800	0.71176000
C	-3.38754700	-0.94747200	-0.03558700
O	-3.23097500	-2.12522500	-0.17243000
N	-1.25230700	-0.16602400	0.98515100
H	-0.78562500	-0.66657100	1.72523500
C	-0.55841700	0.15330100	-0.12561400
O	-1.06452400	0.60228500	-1.13191900
C	0.99219000	0.00892500	-0.04486300
Br	1.68377000	1.80645200	0.40784500
Br	1.60972100	-1.27280000	1.33948900
Br	1.68218100	-0.56302900	-1.77486900
