**Structural Revision of the Product in the Copper-Catalyzed Skeletal Rearrangement of
O-Propargyl Arylaldoximes**

(*J. Am. Chem. Soc.* **2009**, *131*, 2804)

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Contents

Structural Revision

General Information

X-ray Structure Report for Cyclic Nitrone **A**

Computational details

Structural Revision

Introduction

Previously, we reported that the reaction of the *O*-propargylic oxime **1a** in the presence of 10 mol % of CuBr at 100 °C afforded the four-membered cyclic product **2a** and its regioisomer **2a'** in 96% isolated yield (eq 1). At the initial stage, we assigned the products **2a** and **2a'** as the β -lactam **B** and **B'**, respectively, by X-ray crystallographic analysis as reported in *J. Am. Chem. Soc.* **2009**, *131*, 2804. After number of further experiments, however, we noted that the products can be assigned as the four-membered cyclic nitrones **A** and **A'**, respectively. Thus, we reanalyzed the structure of the major product **2a** by X-ray crystallographic analyses and spectral analyses of NMR and IR with DFT calculations.

X-Ray Crystallographic Analyses

The essential difference between the structures of the cyclic nitron **A** and β -lactam **B** is the position of the nitrogen atom in the four-membered ring. Because the carbon and nitrogen atoms have a similar number of electrons, commonly the quaternary carbon and nitrogen can hardly be distinguished by X-ray crystallography. Therefore, we performed a structure determination using X-ray crystallography, and compared them with the results obtained from DFT theoretical calculations.

Single crystals suitable for X-ray structure analysis were obtained by recrystallization from 1,2-dichloroethane/*n*-hexane. X-ray diffraction data were collected at 173 K on a Rigaku Saturn CCD diffractometer with graphite monochromated Mo K α radiation ($\lambda = 0.71070$ Å). The structure was solved by direct methods (SHELX-97)¹ and expanded by using Fourier techniques. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares on F^2 by using the SHELXL-97 crystallographic program package. Hydrogen atoms were placed at calculated positions and refined as riding atoms in the subsequent least-squares model refinements. All hydrogen atoms were assigned fixed isotropic thermal parameters defined as $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{iso}}(\text{parent atom})$. A total of 28460 reflections were measured and 8737 were unique ($R_{\text{int}} = 0.038$). Crystal data and refinement statistics are shown in the X-ray structure reports described below.

The initial geometries of **A** and **B** for the DFT calculations were taken from their X-ray crystallographic structures. The gas phase geometry optimization of the molecules leading to energy minima was achieved using the B3LYP hybrid functional with the 6-311++G(2d,p) basis set as implemented in the Gaussian 03 program package.¹ For all optimized structures, vibrational normal mode analysis was carried out to ensure that the obtained structures were corresponding to minimum energy state.

Fig. S1. (a) Molecular structures and (b) optimized geometries (at B3LYP/6-311++G(2d,p) level of theory) of cyclic nitron **A** and β -lactam **B**.

Table S1. Cartesian coordinates (Angstroms) for **A**.

PG: C1

Total energy = -1430.45826085 hartree

Atom	X	Y	Z
F	-4.9355	-2.55153	-2.11351
F	-6.08052	-1.53163	-0.57884
F	-5.27121	-3.5036	-0.19014
O	7.080362	-0.85058	-0.99034
O	1.09823	-1.98773	1.903127
N	0.983843	-0.86461	1.369738
C	3.789346	-1.48763	0.541445
C	7.783137	-2.05524	-0.70934
C	5.160201	0.475517	-0.8688
C	5.102118	-1.71288	0.149173
C	1.770811	-0.05856	0.649169
C	-1.58575	3.040842	0.775055
C	-0.28984	4.31536	-0.79601
C	-1.28541	5.281065	-0.84305

C	-2.58072	4.006597	0.728154
C	0.74707	0.980667	0.551288
C	-2.8303	-1.08683	-1.10497

Table S2. Cartesian coordinates (Angstroms) for **B**.

PG: C1

Total energy = -1430.53016119 hartree

Atom	X	Y	Z
F	-5.06416	-2.48407	-2.0226
F	-6.09068	-0.91144	-0.94042
F	-5.82891	-2.85889	-0.02373
O	7.087322	-0.74522	-0.81667
O	1.091098	-2.28268	1.890713
N	1.768842	-0.30268	0.76729
C	3.581872	-1.65294	-0.11095
C	7.625598	-1.97232	-1.29166
C	5.306732	0.520296	0.017537
C	4.908407	-1.80131	-0.50242
C	-1.3127	2.994516	0.808363
C	0.938352	-1.16933	1.475573
C	-0.00806	3.984474	-0.94867
C	-0.94324	5.002683	-1.07586
C	-2.24692	4.01302	0.681277
C	0.797131	0.729663	0.67961
C	-2.92228	-0.965	-1.04798
C	0.854506	1.913499	0.063579
C	-1.73017	-0.50225	-0.50956

X-ray crystallographic analysis showed that the structure of the four-membered ring adopted that of the cyclic nitron **A**. Thus, the C atom of the carbonyl group in the structure **B** was distinguished from the N atom on the basis of their isotropic thermal parameters and the bond distances. Although the N-O distances in **A** from 1.2685(19) to 1.2698(19) Å are normal, the lengths of 1.274(3) and 1.271(3) Å for the C=O bonds of **B** are longer than those normally found in the carbonyl group. Moreover, although the R-factors for **B** reached acceptable levels, refinement of the crystal structure for the **A** led to better results than that for **B** (Table S3). A comparison of the other structural parameters of the calculated and the experimental structures also underlines the structure of **A**, as shown **Table S4**.

Table S3. R-factors for cyclic nitron **A** and β -lactam **B**

	Cyclic nitron A	β -Lactam B
R	0.0603	0.0746
wR ₂	0.1783	0.2449
GOF	1.098	1.131

Table S4. Experimental and calculated results in bond lengths and bond angles of **A** and **B** (selected)

Bond lengths (Å)

	Cyclic nitron A (X = N, Y = C)		β -Lactam B (X = C, Y = N)	
	Calculated ^a	Experimental	Calculated ^a	Experimental
X-Y	1.337	1.325	1.394	1.326
Y-C ²	1.462	1.480	1.420	1.473
C ² -C ¹	1.534	1.524	1.529	1.522
C ¹ -X	1.523	1.524	1.559	1.528
O-X	1.249	1.270	1.198	1.271
Y-C ³	1.445	1.448	1.414	1.447

Bond angles

	Cyclic nitron A (X = N, Y = C)		β -Lactam B (X = C, Y = N)	
	Calculated ^a	Experimental	Calculated ^a	Experimental
$\angle$ X-Y-C ²	93.01	92.62	94.34	92.67
$\angle$ Y-C ² -C ¹	89.19	88.86	91.00	89.26

$\angle \text{C}^2\text{-C}^1\text{-X}$	83.34	83.57	83.87	83.32
$\angle \text{C}^1\text{-X-Y}$	94.46	94.92	90.76	94.74
$\angle \text{O-X-Y}$	135.93	134.60	132.69	135.03
$\angle \text{X-Y-C}^3$	128.09	128.59	131.55	128.10
$\angle \text{C}^2\text{-Y-C}^3$	138.88	138.77	134.07	139.22

^a DFT [B3LYP/6-311++G(2d,p)]

NMR Spectral Analysis

Observed C and N NMR chemical shifts of the atoms in the four-membered cycle were compared with computed chemical shifts with the gauge-invariant atomic orbital (GIAO) approach in conjunction with the B3LYP functional theory and the 6-311++G(2d,p) basis set, with initial geometry taken from the crystal structure (Table 3). The absolute shifts (δ) of tetramethylsilane (TMS) for ^{13}C NMR and ammonia (NH_3) for ^{14}N NMR were used to compute the relative chemical shifts. Chemical shifts of the product **2a** in CDCl_3 were reported relative to CDCl_3 (for ^{13}C , δ 77.00) and MeNO_2 (for ^{14}N , 372 ppm). All calculated chemical shifts for the cyclic nitron **A** are in a reasonable accordance with the observed chemical shifts rather than β -lactam **B**. Especially, observed ^{14}N chemical shift at lower fields was reproduced by calculation for the cyclic nitron **A**.

Table S5. Observed and calculated NMR chemical shifts of **2a**, **A**, and **B**.

	C-1	C-2	C-3	^{14}N
Experiment 2a	148.8	129.2	84.9	290.7
Cyclic Nitron A ^a	154.7	136.7	90.7	339.7
β -Lactam B ^a	169.4	145.0	66.8	202.4

^a NMR chemical shifts were calculated using DFT [B3LYP/6-311++G(2d,p)]

Frequency Analysis

Geometry optimization and frequency analysis were carried out using hybrid B3LYP functional theory and the 6-311++G(2d,p) basis set. Calculated results suggest that observed absorption at 1682 cm^{-1} corresponds to absorptions caused by stretching of nitrogen-oxygen bond and carbon-carbon double bond and in-plane skeletal bending of the four membered ring. Carbonyl C=O bond stretching in this β -lactam should be stronger and more than 1800 cm^{-1} .

Figure S2. (a) Observed IR spectrum of **2a**, (b) calculated vibration of the cyclic nitrone **A** and (c) calculated vibration of the β -lactam **B**

Table S6. Observed and calculated vibrational frequencies of **2a**, **A**, and **B**. The notation are ν_1 , stretching of N-O and C=C bond and in-plane skeletal bending of four-membered ring; ν_2 , stretching of C=O and C=C bond and in-plane skeletal bending of four-membered ring.

	ν_1 (A)	ν_2 (B)
experimental	1682	
B3LYP/6-311++G(2d,p)	1726	1851
B3LYP/6-31G(d)	1742	1865

Observed and calculated vibrational frequencies are given in wavenumber (cm^{-1})

Conclusion

Based on these experimental and computational results, it was rationally concluded that the product **2a** is the cyclic nitron A, instead of the β -lactam (eq 2).

Acknowledgment

We thank Dr. Eunsang Kwon (Research and Analytical Center for Giant Molecules, Graduate School of Science, Tohoku University, Japan) for X-ray crystallographic expertise and DFT calculations. ^{14}N NMR spectroscopic experiment was conducted at JEOL LTD.

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General Information

^{13}C NMR spectra were recorded on JEOL ECA-600 (150 MHz for ^{13}C , 43.3 MHz for ^{14}N) spectrometer. Chemical shifts are reported in ppm relative to CDCl_3 (for ^{13}C , δ 77.00) and MeNO_2 (for ^{14}N , 372 ppm). Infrared spectra were recorded on a JASCO FT/IR-4100 spectrometer. X-ray crystallographic data was obtained by Rigaku / MSC Saturn Mo-CCD device at Research and Analytical Center for Giant Molecules, Graduate School of Science, Tohoku University.

X-ray Structure Report for Cyclic Nitron A

Experimental

Data Collection

A colorless prism crystal of $\text{C}_{24}\text{H}_{18}\text{F}_3\text{NO}_2$ having approximate dimensions of 0.290 x 0.170 x 0.060 mm was mounted on a glass fiber. All measurements were made on a Rigaku Saturn70 diffractometer using graphite monochromated $\text{Mo-K}\alpha$ radiation.

The crystal-to-detector distance was 49.38 mm.

Cell constants and an orientation matrix for data collection corresponded to a primitive triclinic cell with dimensions:

$$\begin{array}{ll} a = 9.800(4) \text{ \AA} & \alpha = 79.398(11)^\circ \\ b = 9.819(4) \text{ \AA} & \beta = 80.237(11)^\circ \\ c = 21.005(8) \text{ \AA} & \gamma = 79.763(12)^\circ \\ V = 1935.3(12) \text{ \AA}^3 \end{array}$$

For $Z = 4$ and F.W. = 409.41, the calculated density is 1.405 g/cm^3 . Based on a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

P-1 (#2)

The data were collected at a temperature of $-123 \pm 1^\circ\text{C}$ to a maximum 2θ value of 54.9° . A total of 2400 oscillation images were collected. A sweep of data was done using ω oscillations from -110.0 to 70.0° in 0.3° steps. The exposure rate was $100.0 [\text{sec./}^\circ]$. The detector swing angle was -19.58° . A second sweep

was performed using ω oscillations from -110.0 to 70.0° in 0.3° steps. The exposure rate was 100.0 [sec./ $^\circ$]. The detector swing angle was -19.58° . Another sweep was performed using ω oscillations from -110.0 to 70.0° in 0.3° steps. The exposure rate was 100.0 [sec./ $^\circ$]. The detector swing angle was -19.58° . Another sweep was performed using ω oscillations from -110.0 to 70.0° in 0.3° steps. The exposure rate was 100.0 [sec./ $^\circ$]. The detector swing angle was -19.58° . The crystal-to-detector distance was 49.38 mm. Readout was performed in the 0.137 mm pixel mode.

Data Reduction

Of the 28460 reflections that were collected, 8737 were unique ($R_{\text{int}} = 0.0384$); equivalent reflections were merged. Data were collected and processed using CrystalClear (Rigaku).

The linear absorption coefficient, μ , for Mo-K α radiation is 1.086 cm^{-1} . A numerical absorption correction was applied which resulted in transmission factors ranging from 0.974 to 0.994. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods² and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement³ on F^2 was based on 8737 observed reflections and 541 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o| = 0.0603$$

$$wR2 = [\Sigma (w(F_o^2 - F_c^2)^2) / \Sigma w(F_o^2)^2]^{1/2} = 0.1783$$

The standard deviation of an observation of unit weight⁴ was 1.10. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.57 and $-0.51 \text{ e}^-/\text{\AA}^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber⁵. Anomalous dispersion effects were included in F_{calc} ⁶; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley⁷. The values

for the mass attenuation coefficients are those of Creagh and Hubbell⁸. All calculations were performed using the CrystalStructure⁹ crystallographic software package except for refinement, which was performed using SHELXL-97¹⁰.

References

(1) CrystalClear: Rigaku Corporation, 1999. CrystalClear Software User's Guide, Molecular Structure Corporation, (c) 2000. J.W. Pflugrath (1999) Acta Cryst. D55, 1718-1725.

(2) SHELX97: Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.

(3) Least Squares function minimized: (SHELXL97)

$$\sum w(F_o^2 - F_c^2)^2 \quad \text{where } w = \text{Least Squares weights.}$$

(4) Standard deviation of an observation of unit weight:

$$[\sum w(F_o^2 - F_c^2)^2 / (N_o - N_v)]^{1/2}$$

where: N_o = number of observations

N_v = number of variables

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EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$\text{C}_{24}\text{H}_{18}\text{F}_3\text{NO}_2$
Formula Weight	409.41
Crystal Color, Habit	colorless, prism
Crystal Dimensions	0.290 X 0.170 X 0.060 mm
Crystal System	triclinic
Lattice Type	Primitive
Lattice Parameters	$a = 9.800(4) \text{ \AA}$ $b = 9.819(4) \text{ \AA}$ $c = 21.005(8) \text{ \AA}$ $\alpha = 79.398(11)^\circ$ $\beta = 80.237(11)^\circ$ $\gamma = 79.763(12)^\circ$ $V = 1935.3(12) \text{ \AA}^3$
Space Group	P-1 (#2)
Z value	4
D_{calc}	1.405 g/cm^3
F_{000}	848.00
$\mu(\text{MoK}\alpha)$	1.086 cm^{-1}

B. Intensity Measurements

Diffractometer	Saturn70
Radiation	MoK α ($\lambda = 0.71070 \text{ \AA}$) graphite monochromated
Voltage, Current	50kV, 40mA
Temperature	-123.0°C
Detector Aperture	70 x 70 mm
Data Images	2400 exposures
ω oscillation Range	-110.0 - 70.0°
Exposure Rate	100.0 sec./°
Detector Swing Angle	-19.58°
ω oscillation Range	-110.0 - 70.0°
Exposure Rate	100.0 sec./°
Detector Swing Angle	-19.58°
ω oscillation Range	-110.0 - 70.0°
Exposure Rate	100.0 sec./°
Detector Swing Angle	-19.58°
ω oscillation Range	-110.0 - 70.0°
Exposure Rate	100.0 sec./°

Detector Swing Angle	-19.58°
Detector Position	49.38 mm
Pixel Size	0.137 mm
2 θ _{max}	54.9°
No. of Reflections Measured	Total: 28460 Unique: 8737 ($R_{\text{int}} = 0.0384$)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.974 - 0.994)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SHELX97)
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\sum w (F_o^2 - F_c^2)^2$
Least Squares Weights	$w = 1 / [\sigma^2(F_o^2) + (0.0940 \cdot P)^2 + 0.5827 \cdot P]$ where $P = (\text{Max}(F_o^2, 0) + 2F_c^2)/3$
$2\theta_{\text{max}}$ cutoff	54.9°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	8737
No. Variables	541
Reflection/Parameter Ratio	16.15
Residuals: R1 ($I > 2.00\sigma(I)$)	0.0603
Residuals: R (All reflections)	0.0753
Residuals: wR2 (All reflections)	0.1783
Goodness of Fit Indicator	1.098
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	$0.57 \text{ e}^-/\text{\AA}^3$
Minimum peak in Final Diff. Map	$-0.51 \text{ e}^-/\text{\AA}^3$

Table 1. Atomic coordinates and $B_{\text{iso}}/B_{\text{eq}}$

atom	x	y	z	B_{eq}
F13	0.2191(3)	0.0209(2)	0.48764(8)	7.20(6)
F20	0.1436(2)	0.3067(2)	0.53956(6)	4.95(4)
F29	0.1194(2)	-0.1522(3)	0.53670(8)	7.28(6)
F42	0.3439(2)	0.3359(2)	0.48745(6)	5.30(4)
F46	0.3305(2)	-0.1829(2)	0.49070(7)	5.58(4)
F61	0.1871(3)	0.5122(2)	0.50123(9)	7.71(6)
O2	0.1532(2)	-0.3527(2)	1.11593(6)	2.79(3)
O3	0.2312(2)	0.07369(13)	0.82750(6)	2.79(3)
O8	0.16208(13)	0.1359(2)	1.11933(6)	2.51(3)
O9	0.2085(2)	0.5596(2)	0.82687(6)	2.99(3)
N18	0.3300(2)	-0.0276(2)	0.82087(7)	2.01(3)
N44	0.3180(2)	0.4687(2)	0.82289(7)	2.17(3)
C1	0.1756(2)	-0.1515(2)	1.03046(8)	2.27(3)
C4	0.1719(2)	0.3412(2)	0.95500(9)	2.33(3)
C5	0.7050(2)	-0.2751(2)	0.68906(8)	2.29(3)
C6	0.3749(2)	-0.1438(2)	0.85965(8)	1.97(3)
C7	0.0148(2)	0.1588(3)	1.14490(9)	2.98(4)
C10	0.3471(2)	0.1634(2)	1.03294(8)	2.23(3)
C11	0.2319(2)	-0.1025(2)	0.96677(8)	2.25(3)
C12	0.1170(2)	0.2874(2)	1.01811(9)	2.38(3)
C14	0.8507(2)	-0.3774(2)	0.76995(9)	2.50(3)
C15	0.3704(2)	0.3588(2)	0.86305(8)	2.00(3)
C16	0.2925(2)	-0.3854(2)	1.01505(9)	2.36(3)
C17	0.7441(2)	0.3080(2)	0.70220(9)	2.62(4)
C19	0.7723(2)	0.0616(2)	0.74171(9)	2.48(3)
C21	0.4914(2)	-0.1870(2)	0.80949(8)	1.96(3)
C22	0.8170(2)	-0.3017(2)	0.63955(9)	2.59(4)
C23	0.8685(2)	0.0366(2)	0.68636(10)	3.04(4)
C24	0.8410(2)	0.2825(3)	0.64691(10)	3.07(4)
C25	0.9465(2)	-0.3669(2)	0.65520(10)	2.75(4)
C26	0.9632(2)	-0.4032(2)	0.72035(10)	2.91(4)
C27	0.4917(2)	0.3223(2)	0.81353(8)	2.01(3)
C28	0.6038(2)	-0.2870(2)	0.80907(8)	2.06(3)

C30	0.2442(2)	0.3236(2)	0.65164(9)	2.31(3)
C31	0.5991(2)	0.2169(2)	0.80837(8)	2.04(3)
C32	0.4423(2)	-0.0554(2)	0.76251(8)	2.03(3)
C33	0.0531(2)	-0.2643(3)	1.15590(9)	3.03(4)

Table 1. Atomic coordinates and $B_{\text{iso}}/B_{\text{eq}}$ (continued)

atom	x	y	z	B_{eq}
C34	0.2940(2)	0.3363(2)	0.70784(8)	2.12(3)
C35	0.7195(2)	-0.3119(2)	0.75482(8)	1.98(3)
C36	0.3858(2)	-0.0667(2)	0.70209(8)	2.00(3)
C37	0.2861(2)	-0.1536(2)	0.70431(9)	2.35(3)
C38	0.9028(2)	0.1459(3)	0.63848(10)	3.14(4)
C39	0.4340(2)	0.0111(2)	0.64281(9)	2.43(3)
C41	0.4010(2)	0.2161(2)	0.97011(8)	2.10(3)
C43	0.7055(2)	0.1974(2)	0.75030(8)	2.08(3)
C45	0.3188(2)	-0.1937(2)	0.92645(8)	1.94(3)
C47	0.4364(2)	0.4497(2)	0.76647(8)	2.07(3)
C48	0.2902(2)	0.4022(2)	0.59266(8)	2.23(3)
C49	0.3886(2)	0.4291(2)	0.70494(8)	1.98(3)
C50	0.2043(2)	0.1969(2)	1.05734(8)	2.03(3)
C51	0.3857(2)	0.4935(2)	0.58908(9)	2.58(4)
C52	0.2863(2)	-0.0856(2)	0.58855(9)	2.59(4)
C53	0.3139(2)	0.3059(2)	0.92949(8)	2.03(3)
C54	0.3851(2)	0.0014(2)	0.58605(9)	2.71(4)
C55	0.3481(2)	-0.3359(2)	0.95176(8)	2.21(3)
C56	0.2399(2)	0.3910(2)	0.53079(9)	2.87(4)
C57	0.2368(2)	-0.1631(2)	0.64754(9)	2.58(4)
C58	0.4340(2)	0.5070(2)	0.64555(9)	2.51(4)
C59	0.2044(2)	-0.2936(2)	1.05474(8)	2.18(3)
C60	0.2373(3)	-0.0987(3)	0.52670(10)	3.26(4)

$$B_{\text{eq}} = 8/3 \pi^2 (U_{11}(\text{aa}^*)^2 + U_{22}(\text{bb}^*)^2 + U_{33}(\text{cc}^*)^2 + 2U_{12}(\text{aa}^*\text{bb}^*)\cos \gamma + 2U_{13}(\text{aa}^*\text{cc}^*)\cos \beta + 2U_{23}(\text{bb}^*\text{cc}^*)\cos \alpha)$$

Table 2. Atomic coordinates and B_{iso} involving hydrogen atoms

atom	x	y	z	B_{iso}
H1	0.1182	-0.0889	1.0570	2.72
H4	0.1118	0.4039	0.9281	2.80
H5	0.6166	-0.2306	0.6772	2.75
H7A	-0.0386	0.1238	1.1176	3.58
H7B	-0.0169	0.2593	1.1447	3.58
H7C	0.0000	0.1088	1.1898	3.58
H10	0.4077	0.1031	1.0604	2.67
H11	0.2116	-0.0056	0.9499	2.70
H12	0.0208	0.3125	1.0340	2.86
H14	0.8644	-0.4050	0.8145	3.00
H16	0.3136	-0.4821	1.0321	2.83
H17	0.7042	0.4017	0.7071	3.15
H19	0.7514	-0.0153	0.7745	2.97
H22	0.8036	-0.2748	0.5950	3.11
H23	0.9106	-0.0566	0.6818	3.65
H24	0.8651	0.3590	0.6146	3.68
H25	1.0224	-0.3863	0.6219	3.29
H26	1.0523	-0.4465	0.7319	3.50
H28	0.6104	-0.3507	0.8488	2.47
H30	0.1791	0.2614	0.6536	2.78
H31	0.6078	0.1474	0.8460	2.45
H32	0.5103	0.0130	0.7533	2.43
H33A	0.0962	-0.1859	1.1622	3.63
H33B	0.0251	-0.3194	1.1985	3.63
H33C	-0.0296	-0.2279	1.1340	3.63
H34	0.2638	0.2820	0.7484	2.54
H37	0.2521	-0.2061	0.7448	2.82
H38	0.9671	0.1290	0.6005	3.76
H39	0.5009	0.0712	0.6413	2.92
H41	0.4974	0.1911	0.9545	2.52
H47	0.4967	0.5250	0.7582	2.48
H51	0.4174	0.5462	0.5483	3.10
H54	0.4189	0.0539	0.5456	3.25

H55	0.4062	-0.3986	0.9255	2.65
H57	0.1694	-0.2226	0.6489	3.09
H58	0.4985	0.5698	0.6435	3.01

Table 3. Anisotropic displacement parameters

atom	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
F13	0.170(2)	0.0523(9)	0.0633(10)	-0.0093(11)	-0.0752(12)	0.0067(8)
F20	0.0579(9)	0.1044(12)	0.0385(7)	-0.0440(9)	-0.0103(6)	-0.0106(7)
F29	0.0744(11)	0.173(2)	0.0471(9)	-0.0625(13)	-0.0235(8)	-0.0062(10)
F42	0.0521(9)	0.125(2)	0.0360(7)	-0.0272(9)	0.0019(6)	-0.0357(8)
F46	0.0829(12)	0.0849(12)	0.0498(9)	0.0055(9)	-0.0211(8)	-0.0318(8)
F61	0.177(2)	0.0524(10)	0.0799(12)	0.0023(11)	-0.094(2)	-0.0007(8)
O2	0.0361(7)	0.0361(8)	0.0281(7)	-0.0017(6)	0.0030(6)	-0.0010(6)
O3	0.0357(7)	0.0275(7)	0.0365(7)	0.0038(6)	0.0010(6)	-0.0022(6)
O8	0.0264(7)	0.0411(8)	0.0260(7)	-0.0048(6)	-0.0016(5)	-0.0022(6)
O9	0.0394(8)	0.0355(8)	0.0326(7)	0.0101(6)	-0.0057(6)	-0.0046(6)
N18	0.0249(7)	0.0248(7)	0.0258(7)	-0.0037(6)	-0.0011(6)	-0.0041(6)
N44	0.0311(8)	0.0268(8)	0.0245(7)	-0.0007(6)	-0.0060(6)	-0.0057(6)
C1	0.0281(9)	0.0307(9)	0.0281(9)	-0.0039(7)	-0.0019(7)	-0.0090(7)
C4	0.0279(9)	0.0312(9)	0.0310(9)	-0.0028(7)	-0.0093(7)	-0.0057(7)
C5	0.0261(9)	0.0304(9)	0.0315(9)	-0.0019(7)	-0.0065(7)	-0.0072(7)
C6	0.0238(8)	0.0255(9)	0.0267(9)	-0.0043(7)	-0.0055(7)	-0.0048(7)
C7	0.0267(9)	0.0511(12)	0.0345(10)	-0.0079(9)	0.0018(8)	-0.0076(9)
C10	0.0249(9)	0.0323(9)	0.0282(9)	-0.0024(7)	-0.0092(7)	-0.0038(7)
C11	0.0290(9)	0.0274(9)	0.0302(9)	-0.0039(7)	-0.0072(7)	-0.0055(7)
C12	0.0243(9)	0.0351(10)	0.0326(9)	-0.0034(7)	-0.0048(7)	-0.0094(8)
C14	0.0311(10)	0.0297(9)	0.0346(10)	-0.0020(8)	-0.0098(8)	-0.0043(8)
C15	0.0275(9)	0.0246(9)	0.0259(9)	-0.0041(7)	-0.0071(7)	-0.0055(7)
C16	0.0314(9)	0.0279(9)	0.0309(9)	-0.0062(7)	-0.0053(7)	-0.0034(7)
C17	0.0314(10)	0.0290(9)	0.0376(10)	-0.0051(8)	-0.0042(8)	-0.0009(8)
C19	0.0256(9)	0.0314(10)	0.0382(10)	-0.0072(7)	-0.0060(8)	-0.0040(8)
C21	0.0260(9)	0.0270(9)	0.0241(8)	-0.0076(7)	-0.0060(7)	-0.0051(7)
C22	0.0358(10)	0.0328(10)	0.0316(10)	-0.0065(8)	-0.0056(8)	-0.0072(8)
C23	0.0292(10)	0.0335(10)	0.0537(13)	-0.0060(8)	-0.0001(9)	-0.0136(9)
C24	0.0380(11)	0.0418(11)	0.0344(10)	-0.0112(9)	-0.0009(8)	0.0010(9)
C25	0.0308(10)	0.0330(10)	0.0396(11)	-0.0052(8)	0.0033(8)	-0.0105(8)
C26	0.0261(9)	0.0362(11)	0.0463(11)	0.0008(8)	-0.0045(8)	-0.0071(9)
C27	0.0275(9)	0.0280(9)	0.0228(8)	-0.0076(7)	-0.0056(7)	-0.0037(7)
C28	0.0263(9)	0.0275(9)	0.0259(9)	-0.0055(7)	-0.0058(7)	-0.0044(7)

C30	0.0290(9)	0.0294(9)	0.0304(9)	-0.0063(7)	-0.0059(7)	-0.0037(7)
C31	0.0266(9)	0.0264(9)	0.0257(9)	-0.0062(7)	-0.0060(7)	-0.0023(7)
C32	0.0226(8)	0.0265(9)	0.0276(9)	-0.0052(7)	-0.0014(7)	-0.0037(7)
C33	0.0377(11)	0.0457(12)	0.0276(10)	-0.0020(9)	0.0022(8)	-0.0061(8)

Table 3. Anisotropic displacement parameters (continued)

atom	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C34	0.0293(9)	0.0263(9)	0.0237(8)	-0.0052(7)	-0.0029(7)	-0.0007(7)
C35	0.0243(8)	0.0222(8)	0.0304(9)	-0.0054(7)	-0.0044(7)	-0.0058(7)
C36	0.0232(8)	0.0253(9)	0.0256(8)	-0.0005(7)	-0.0021(7)	-0.0029(7)
C37	0.0273(9)	0.0326(10)	0.0284(9)	-0.0071(7)	-0.0029(7)	-0.0007(7)
C38	0.0346(11)	0.0464(12)	0.0380(11)	-0.0094(9)	0.0046(8)	-0.0120(9)
C39	0.0316(10)	0.0283(9)	0.0312(9)	-0.0074(8)	-0.0029(8)	-0.0000(7)
C41	0.0229(8)	0.0294(9)	0.0278(9)	-0.0033(7)	-0.0049(7)	-0.0046(7)
C43	0.0241(8)	0.0299(9)	0.0275(9)	-0.0064(7)	-0.0076(7)	-0.0049(7)
C45	0.0225(8)	0.0281(9)	0.0249(8)	-0.0061(7)	-0.0055(7)	-0.0046(7)
C47	0.0292(9)	0.0254(9)	0.0244(8)	-0.0047(7)	-0.0036(7)	-0.0048(7)
C48	0.0273(9)	0.0332(10)	0.0244(9)	-0.0024(7)	-0.0043(7)	-0.0064(7)
C49	0.0262(8)	0.0236(8)	0.0251(8)	-0.0010(7)	-0.0048(7)	-0.0042(7)
C50	0.0269(9)	0.0292(9)	0.0237(8)	-0.0082(7)	-0.0037(7)	-0.0073(7)
C51	0.0391(10)	0.0336(10)	0.0254(9)	-0.0108(8)	-0.0036(8)	-0.0005(7)
C52	0.0338(10)	0.0340(10)	0.0297(10)	0.0005(8)	-0.0086(8)	-0.0044(8)
C53	0.0287(9)	0.0267(9)	0.0245(8)	-0.0060(7)	-0.0065(7)	-0.0064(7)
C54	0.0396(11)	0.0330(10)	0.0266(9)	-0.0063(8)	-0.0008(8)	0.0018(8)
C55	0.0267(9)	0.0279(9)	0.0298(9)	-0.0037(7)	-0.0027(7)	-0.0075(7)
C56	0.0402(11)	0.0417(11)	0.0285(10)	-0.0078(9)	-0.0089(8)	-0.0037(8)
C57	0.0287(9)	0.0361(10)	0.0344(10)	-0.0087(8)	-0.0067(8)	-0.0030(8)
C58	0.0355(10)	0.0320(10)	0.0296(9)	-0.0136(8)	-0.0062(8)	0.0002(8)
C59	0.0249(9)	0.0330(10)	0.0256(9)	-0.0066(7)	-0.0040(7)	-0.0039(7)
C60	0.0476(12)	0.0440(12)	0.0331(11)	-0.0053(10)	-0.0137(9)	-0.0026(9)

The general temperature factor expression: $\exp(-2\pi^2(a^2U_{11}h^2 + b^2U_{22}k^2 + c^2U_{33}l^2 + 2a*b*U_{12}hk + 2a*c*U_{13}hl + 2b*c*U_{23}kl))$

Table 4. Fragment Analysis

fragment: 1

F(13)	F(29)	F(46)	O(2)	O(3)
N(18)	C(1)	C(5)	C(6)	C(11)
C(14)	C(16)	C(21)	C(22)	C(25)
C(26)	C(28)	C(32)	C(33)	C(35)
C(36)	C(37)	C(39)	C(45)	C(52)
C(54)	C(55)	C(57)	C(59)	C(60)

fragment: 2

F(20)	F(42)	F(61)	O(8)	O(9)
N(44)	C(4)	C(7)	C(10)	C(12)
C(15)	C(17)	C(19)	C(23)	C(24)
C(27)	C(30)	C(31)	C(34)	C(38)
C(41)	C(43)	C(47)	C(48)	C(49)
C(50)	C(51)	C(53)	C(56)	C(58)

Table 5. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
F13	C60	1.306(3)	F20	C56	1.331(3)
F29	C60	1.322(4)	F42	C56	1.354(3)
F46	C60	1.348(3)	F61	C56	1.299(3)
O2	C33	1.451(3)	O2	C59	1.361(2)
O3	N18	1.2685(19)	O8	C7	1.445(3)
O8	C50	1.358(2)	O9	N44	1.2698(19)
N18	C6	1.326(2)	N18	C32	1.532(2)
N44	C15	1.325(2)	N44	C47	1.524(3)
C1	C11	1.390(3)	C1	C59	1.390(3)
C4	C12	1.388(3)	C4	C53	1.409(3)
C5	C22	1.402(3)	C5	C35	1.387(3)
C6	C21	1.476(3)	C6	C45	1.446(3)
C10	C41	1.378(3)	C10	C50	1.409(3)
C11	C45	1.417(3)	C12	C50	1.378(3)
C14	C26	1.405(3)	C14	C35	1.392(3)
C15	C27	1.480(3)	C15	C53	1.448(3)
C16	C55	1.382(3)	C16	C59	1.418(3)
C17	C24	1.400(3)	C17	C43	1.399(3)
C19	C23	1.397(3)	C19	C43	1.406(3)
C21	C28	1.339(3)	C21	C32	1.531(3)
C22	C25	1.380(3)	C23	C38	1.375(3)
C24	C38	1.400(3)	C25	C26	1.379(3)
C27	C31	1.344(3)	C27	C47	1.524(3)
C28	C35	1.487(3)	C30	C34	1.385(3)
C30	C48	1.384(3)	C31	C43	1.481(3)
C32	C36	1.497(3)	C34	C49	1.398(3)
C36	C37	1.397(3)	C36	C39	1.391(3)
C37	C57	1.384(3)	C39	C54	1.383(3)
C41	C53	1.392(3)	C45	C55	1.397(3)
C47	C49	1.505(3)	C48	C51	1.391(3)
C48	C56	1.494(3)	C49	C58	1.385(3)
C51	C58	1.385(3)	C52	C54	1.389(3)
C52	C57	1.389(3)	C52	C60	1.493(4)

Table 6. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C1	H1	0.950	C4	H4	0.950
C5	H5	0.950	C7	H7A	0.980
C7	H7B	0.980	C7	H7C	0.980
C10	H10	0.950	C11	H11	0.950
C12	H12	0.950	C14	H14	0.950
C16	H16	0.950	C17	H17	0.950
C19	H19	0.950	C22	H22	0.950
C23	H23	0.950	C24	H24	0.950
C25	H25	0.950	C26	H26	0.950
C28	H28	0.950	C30	H30	0.950
C31	H31	0.950	C32	H32	1.000
C33	H33A	0.980	C33	H33B	0.980
C33	H33C	0.980	C34	H34	0.950
C37	H37	0.950	C38	H38	0.950
C39	H39	0.950	C41	H41	0.950
C47	H47	1.000	C51	H51	0.950
C54	H54	0.950	C55	H55	0.950
C57	H57	0.950	C58	H58	0.950

Table 7. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
C33	O2	C59	117.83(14)	C7	O8	C50	118.53(14)
O3	N18	C6	134.36(14)	O3	N18	C32	130.82(13)
C6	N18	C32	94.81(13)	O9	N44	C15	134.60(14)
O9	N44	C47	130.48(13)	C15	N44	C47	94.92(13)
C11	C1	C59	119.05(16)	C12	C4	C53	122.28(16)
C22	C5	C35	121.93(16)	N18	C6	C21	92.92(13)
N18	C6	C45	128.49(15)	C21	C6	C45	138.58(14)
C41	C10	C50	121.53(16)	C1	C11	C45	121.53(15)
C4	C12	C50	118.93(16)	C26	C14	C35	120.97(18)
N44	C15	C27	92.62(13)	N44	C15	C53	128.59(15)
C27	C15	C53	138.77(15)	C55	C16	C59	120.75(16)
C24	C17	C43	120.84(18)	C23	C19	C43	121.89(16)
C6	C21	C28	134.84(15)	C6	C21	C32	89.03(12)
C28	C21	C32	135.44(15)	C5	C22	C25	120.40(18)
C19	C23	C38	120.54(18)	C17	C24	C38	121.04(18)
C22	C25	C26	118.49(17)	C14	C26	C25	121.10(18)
C15	C27	C31	136.69(15)	C15	C27	C47	88.86(13)
C31	C27	C47	134.21(15)	C21	C28	C35	128.70(15)
C34	C30	C48	119.45(19)	C27	C31	C43	127.03(15)
N18	C32	C21	83.22(11)	N18	C32	C36	114.47(14)
C21	C32	C36	120.80(16)	C30	C34	C49	120.11(15)
C5	C35	C14	117.11(15)	C5	C35	C28	123.96(15)
C14	C35	C28	118.93(16)	C32	C36	C37	121.20(15)
C32	C36	C39	119.07(17)	C37	C36	C39	119.73(18)
C36	C37	C57	119.97(16)	C23	C38	C24	118.62(18)
C36	C39	C54	120.31(19)	C10	C41	C53	119.88(15)
C17	C43	C19	117.02(15)	C17	C43	C31	123.46(16)
C19	C43	C31	119.52(15)	C6	C45	C11	121.74(15)
C6	C45	C55	119.48(15)	C11	C45	C55	118.77(15)
N44	C47	C27	83.57(12)	N44	C47	C49	113.89(15)
C27	C47	C49	119.56(16)	C30	C48	C51	120.92(18)
C30	C48	C56	121.22(19)	C51	C48	C56	117.86(16)
C34	C49	C47	120.27(14)	C34	C49	C58	119.83(18)

C47	C49	C58	119.84(17)	O8	C50	C10	116.43(15)
O8	C50	C12	124.23(15)	C10	C50	C12	119.34(15)
C48	C51	C58	119.39(17)	C54	C52	C57	120.5(2)
C54	C52	C60	119.25(17)	C57	C52	C60	120.2(2)

Table 7. Bond angles ($^{\circ}$) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C4	C53	C15	122.31(15)	C4	C53	C41	118.01(15)
C15	C53	C41	119.67(15)	C39	C54	C52	119.67(17)
C16	C55	C45	120.03(16)	F20	C56	F42	104.24(19)
F20	C56	F61	107.4(2)	F20	C56	C48	113.53(15)
F42	C56	F61	106.72(17)	F42	C56	C48	112.26(17)
F61	C56	C48	112.1(2)	C37	C57	C52	119.8(2)
C49	C58	C51	120.29(19)	O2	C59	C1	123.82(16)
O2	C59	C16	116.33(16)	C1	C59	C16	119.85(15)
F13	C60	F29	107.9(2)	F13	C60	F46	104.45(17)
F13	C60	C52	112.6(2)	F29	C60	F46	105.4(3)
F29	C60	C52	113.24(17)	F46	C60	C52	112.67(18)

Table 8. Bond angles involving hydrogens ($^{\circ}$)

atom	atom	atom	angle	atom	atom	atom	angle
C11	C1	H1	120	C59	C1	H1	120
C12	C4	H4	119	C53	C4	H4	119
C22	C5	H5	119	C35	C5	H5	119
O8	C7	H7A	109	O8	C7	H7B	109
O8	C7	H7C	109	H7A	C7	H7B	109
H7A	C7	H7C	109	H7B	C7	H7C	109
C41	C10	H10	119	C50	C10	H10	119
C1	C11	H11	119	C45	C11	H11	119
C4	C12	H12	121	C50	C12	H12	121
C26	C14	H14	120	C35	C14	H14	120
C55	C16	H16	120	C59	C16	H16	120
C24	C17	H17	120	C43	C17	H17	120
C23	C19	H19	119	C43	C19	H19	119
C5	C22	H22	120	C25	C22	H22	120
C19	C23	H23	120	C38	C23	H23	120
C17	C24	H24	119	C38	C24	H24	119
C22	C25	H25	121	C26	C25	H25	121
C14	C26	H26	119	C25	C26	H26	119
C21	C28	H28	116	C35	C28	H28	116
C34	C30	H30	120	C48	C30	H30	120
C27	C31	H31	116	C43	C31	H31	116
N18	C32	H32	112	C21	C32	H32	112
C36	C32	H32	112	O2	C33	H33A	109
O2	C33	H33B	109	O2	C33	H33C	109
H33A	C33	H33B	109	H33A	C33	H33C	109
H33B	C33	H33C	109	C30	C34	H34	120
C49	C34	H34	120	C36	C37	H37	120
C57	C37	H37	120	C23	C38	H38	121
C24	C38	H38	121	C36	C39	H39	120
C54	C39	H39	120	C10	C41	H41	120
C53	C41	H41	120	N44	C47	H47	112
C27	C47	H47	112	C49	C47	H47	112
C48	C51	H51	120	C58	C51	H51	120

C39	C54	H54	120	C52	C54	H54	120
C16	C55	H55	120	C45	C55	H55	120
C37	C57	H57	120	C52	C57	H57	120
C49	C58	H58	120	C51	C58	H58	120

Table 8. Bond angles involving hydrogens ($^{\circ}$) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
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Table 9. Torsion Angles($^{\circ}$)(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C33	O2	C59	C1	5.6(3)	C33	O2	C59	C16	-174.80(16)
C7	O8	C50	C10	-175.58(16)	C7	O8	C50	C12	4.4(3)
O3	N18	C6	C21	-178.7(2)	O3	N18	C6	C45	0.5(4)
O3	N18	C32	C21	178.71(19)	O3	N18	C32	C36	-60.5(3)
C6	N18	C32	C21	-0.85(14)	C6	N18	C32	C36	119.98(15)
C32	N18	C6	C21	0.87(14)	C32	N18	C6	C45	-179.96(18)
O9	N44	C15	C27	178.0(2)	O9	N44	C15	C53	-0.7(4)
O9	N44	C47	C27	-178.08(19)	O9	N44	C47	C49	-58.5(3)
C15	N44	C47	C27	1.14(14)	C15	N44	C47	C49	120.68(15)
C47	N44	C15	C27	-1.17(14)	C47	N44	C15	C53	-179.86(18)
C11	C1	C59	O2	-179.09(17)	C11	C1	C59	C16	1.3(3)
C59	C1	C11	C45	-0.6(3)	C12	C4	C53	C15	178.19(18)
C12	C4	C53	C41	-1.3(3)	C53	C4	C12	C50	0.3(3)
C22	C5	C35	C14	-0.2(3)	C22	C5	C35	C28	-179.45(16)
C35	C5	C22	C25	0.3(3)	N18	C6	C21	C28	170.4(2)
N18	C6	C21	C32	-0.87(14)	N18	C6	C45	C11	-19.9(3)
N18	C6	C45	C55	158.66(18)	C21	C6	C45	C11	158.9(2)
C21	C6	C45	C55	-22.6(4)	C45	C6	C21	C28	-8.6(4)
C45	C6	C21	C32	-179.9(3)	C41	C10	C50	O8	178.23(17)
C41	C10	C50	C12	-1.7(3)	C50	C10	C41	C53	0.8(3)
C1	C11	C45	C6	178.48(16)	C1	C11	C45	C55	-0.1(3)
C4	C12	C50	O8	-178.79(18)	C4	C12	C50	C10	1.2(3)
C26	C14	C35	C5	0.7(3)	C26	C14	C35	C28	179.92(16)
C35	C14	C26	C25	-1.2(3)	N44	C15	C27	C31	-173.6(3)
N44	C15	C27	C47	1.17(14)	N44	C15	C53	C4	19.2(4)
N44	C15	C53	C41	-161.37(18)	C27	C15	C53	C4	-158.8(2)
C27	C15	C53	C41	20.6(4)	C53	C15	C27	C31	4.9(5)
C53	C15	C27	C47	179.6(3)	C55	C16	C59	O2	179.02(17)
C55	C16	C59	C1	-1.4(3)	C59	C16	C55	C45	0.7(3)
C24	C17	C43	C19	2.5(3)	C24	C17	C43	C31	-177.19(18)
C43	C17	C24	C38	-0.6(4)	C23	C19	C43	C17	-2.7(3)
C23	C19	C43	C31	176.96(17)	C43	C19	C23	C38	1.0(3)

C6	C21	C28	C35	-175.19(18)	C6	C21	C32	N18	0.76(12)
C6	C21	C32	C36	-113.74(15)	C28	C21	C32	N18	-170.4(3)
C28	C21	C32	C36	75.1(3)	C32	C21	C28	C35	-7.7(4)
C5	C22	C25	C26	-0.8(3)	C19	C23	C38	C24	1.0(4)
C17	C24	C38	C23	-1.2(4)	C22	C25	C26	C14	1.3(3)

Table 9. Torsion angles ($^{\circ}$) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C15	C27	C31	C43	175.1(2)	C15	C27	C47	N44	-1.02(13)
C15	C27	C47	C49	-114.88(15)	C31	C27	C47	N44	174.0(3)
C31	C27	C47	C49	60.1(3)	C47	C27	C31	C43	2.4(4)
C21	C28	C35	C5	-28.1(3)	C21	C28	C35	C14	152.75(19)
C34	C30	C48	C51	0.1(3)	C34	C30	C48	C56	179.63(14)
C48	C30	C34	C49	0.7(3)	C27	C31	C43	C17	26.2(3)
C27	C31	C43	C19	-153.47(19)	N18	C32	C36	C37	-49.81(19)
N18	C32	C36	C39	130.22(14)	C21	C32	C36	C37	47.1(2)
C21	C32	C36	C39	-132.88(14)	C30	C34	C49	C47	176.36(13)
C30	C34	C49	C58	-0.9(3)	C32	C36	C37	C57	-179.29(13)
C32	C36	C39	C54	179.15(13)	C37	C36	C39	C54	-0.8(3)
C39	C36	C37	C57	0.7(3)	C36	C37	C57	C52	-0.3(3)
C36	C39	C54	C52	0.6(3)	C10	C41	C53	C4	0.7(3)
C10	C41	C53	C15	-178.76(17)	C6	C45	C55	C16	-178.53(16)
C11	C45	C55	C16	0.0(3)	N44	C47	C49	C34	-45.70(19)
N44	C47	C49	C58	131.52(14)	C27	C47	C49	C34	50.6(2)
C27	C47	C49	C58	-132.15(15)	C30	C48	C51	C58	-0.7(3)
C30	C48	C56	F20	3.7(3)	C30	C48	C56	F42	-114.23(18)
C30	C48	C56	F61	125.62(18)	C51	C48	C56	F20	-176.74(15)
C51	C48	C56	F42	65.3(2)	C51	C48	C56	F61	-54.8(2)
C56	C48	C51	C58	179.68(14)	C34	C49	C58	C51	0.2(3)
C47	C49	C58	C51	-177.05(13)	C48	C51	C58	C49	0.6(3)
C54	C52	C57	C37	0.1(3)	C57	C52	C54	C39	-0.3(3)
C54	C52	C60	F13	-40.2(3)	C54	C52	C60	F29	-162.88(16)
C54	C52	C60	F46	77.6(3)	C60	C52	C54	C39	-178.16(15)
C57	C52	C60	F13	141.88(17)	C57	C52	C60	F29	19.2(3)
C57	C52	C60	F46	-100.3(2)	C60	C52	C57	C37	178.00(15)

Table 10. Intramolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
F13	C54	2.800(4)	F13	C57	3.526(3)
F20	C30	2.745(3)	F29	C57	2.744(3)
F42	C30	3.407(3)	F42	C51	2.976(3)
F46	C54	3.101(3)	F46	C57	3.299(3)
F61	C30	3.435(3)	F61	C51	2.862(4)
O3	C11	3.113(3)	O3	C21	3.302(3)
O3	C36	3.221(3)	O3	C45	3.122(2)
O9	C4	3.130(3)	O9	C27	3.300(3)
O9	C34	3.523(3)	O9	C49	3.192(3)
O9	C53	3.128(3)	N18	C11	3.046(3)
N18	C28	3.365(3)	N18	C37	3.061(3)
N44	C4	3.054(3)	N44	C31	3.372(3)
N44	C34	3.007(3)	C1	C33	2.817(3)
C1	C55	2.816(3)	C4	C10	2.741(3)
C5	C21	3.146(3)	C5	C26	2.747(3)
C5	C32	3.401(3)	C5	C36	3.419(3)
C6	C36	3.244(3)	C6	C37	3.539(3)
C7	C12	2.828(3)	C11	C16	2.771(3)
C12	C41	2.805(3)	C14	C22	2.763(3)
C15	C34	3.520(3)	C15	C49	3.246(3)
C17	C23	2.781(3)	C17	C27	3.105(3)
C17	C47	3.267(3)	C17	C49	3.470(3)
C17	C58	3.568(3)	C19	C24	2.756(3)
C21	C37	3.169(3)	C21	C55	3.277(3)
C25	C35	2.834(3)	C27	C34	3.155(3)
C27	C41	3.282(3)	C28	C36	3.534(3)
C28	C45	3.508(3)	C28	C55	3.584(3)
C30	C58	2.782(3)	C31	C49	3.412(3)
C31	C53	3.548(3)	C32	C35	3.364(3)
C32	C45	3.552(3)	C34	C51	2.780(3)
C36	C52	2.773(3)	C37	C54	2.783(3)
C38	C43	2.839(3)	C39	C57	2.779(3)
C43	C47	3.300(3)	C45	C59	2.806(3)

C47	C53	3.548(3)	C48	C49	2.767(3)
C50	C53	2.808(3)			

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
F13	H54	2.568	F20	H30	2.427
F29	H57	2.439	F42	H30	3.590
F42	H51	2.868	F46	H54	3.086
F46	H57	3.413	F61	H51	2.707
O2	H1	2.647	O2	H16	2.522
O3	H11	2.530	O3	H32	2.929
O3	H37	3.471	O8	H10	2.508
O8	H12	2.642	O9	H4	2.528
O9	H34	3.356	O9	H47	2.938
N18	H11	2.793	N18	H37	2.851
N44	H4	2.792	N44	H34	2.788
C1	H16	3.283	C1	H33A	2.720
C1	H33C	2.790	C4	H41	3.266
C5	H14	3.234	C5	H25	3.276
C5	H28	3.307	C5	H32	3.475
C6	H11	2.672	C6	H28	2.799
C6	H32	2.752	C6	H37	3.072
C6	H55	2.620	C7	H12	2.530
C10	H12	3.271	C11	H55	3.284
C12	H7A	2.797	C12	H7B	2.746
C12	H10	3.258	C14	H5	3.232
C14	H25	3.284	C14	H28	2.641
C15	H4	2.671	C15	H31	2.850
C15	H34	3.043	C15	H41	2.621
C15	H47	2.741	C16	H1	3.292
C17	H19	3.251	C17	H31	3.321
C17	H38	3.296	C17	H47	3.150
C17	H58	3.400	C19	H17	3.256
C19	H31	2.666	C19	H38	3.269
C21	H5	2.916	C21	H37	2.952
C21	H55	3.002	C22	H26	3.230
C23	H24	3.243	C24	H23	3.248
C25	H5	3.262	C25	H14	3.273

C26	H22	3.232	C27	H17	2.880
C27	H34	2.927	C27	H41	3.010
C28	H5	2.708	C28	H14	2.622
C28	H32	3.004	C28	H55	3.015

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C30	H51	3.270	C31	H17	2.716
C31	H19	2.638	C31	H41	3.041
C31	H47	3.062	C32	H5	2.852
C32	H28	3.433	C32	H37	2.686
C32	H39	2.636	C33	H1	2.513
C34	H47	3.353	C34	H58	3.267
C35	H22	3.287	C35	H26	3.284
C35	H32	3.470	C36	H5	2.567
C36	H54	3.265	C36	H57	3.267
C37	H5	3.169	C37	H32	3.350
C37	H39	3.269	C38	H17	3.289
C38	H19	3.256	C39	H5	2.766
C39	H32	2.561	C39	H37	3.269
C41	H4	3.256	C41	H31	3.118
C43	H23	3.300	C43	H24	3.285
C43	H47	3.508	C45	H1	3.307
C45	H16	3.263	C45	H28	3.314
C47	H17	2.708	C47	H31	3.432
C47	H34	2.674	C47	H58	2.652
C48	H34	3.250	C48	H58	3.256
C49	H17	3.063	C49	H30	3.271
C49	H51	3.262	C50	H4	3.236
C50	H7A	2.652	C50	H7B	2.652
C50	H7C	3.215	C50	H41	3.287
C51	H30	3.271	C52	H37	3.259
C52	H39	3.255	C53	H10	3.251
C53	H12	3.305	C53	H31	3.390
C54	H5	3.469	C54	H57	3.268
C55	H11	3.276	C55	H28	3.067
C56	H30	2.677	C56	H51	2.617
C57	H54	3.269	C58	H17	3.074
C58	H34	3.265	C58	H47	2.588
C59	H11	3.252	C59	H33A	2.647

C59	H33B	3.217	C59	H33C	2.649
C59	H55	3.291	C60	H54	2.641
C60	H57	2.659	H1	H11	2.336
H1	H33A	2.230	H1	H33B	3.483

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H1	H33C	2.382	H4	H12	2.330
H5	H22	2.335	H5	H28	3.573
H5	H32	3.052	H5	H37	3.595
H5	H39	2.985	H7A	H12	2.386
H7B	H12	2.268	H7C	H12	3.502
H10	H41	2.317	H14	H26	2.340
H14	H28	2.462	H16	H55	2.327
H17	H24	2.337	H17	H31	3.587
H17	H47	2.370	H17	H58	2.737
H19	H23	2.329	H19	H31	2.482
H22	H25	2.338	H23	H38	2.331
H24	H38	2.352	H25	H26	2.332
H28	H55	2.405	H30	H34	2.338
H31	H41	2.430	H32	H39	2.331
H37	H57	2.336	H39	H54	2.333
H47	H58	2.366	H51	H58	2.338

Table 12. Intermolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
F13	F20	3.118(3)	F13	F29 ¹	3.426(3)
F13	F42	3.521(3)	F13	C22 ²	3.483(3)
F20	F13	3.118(3)	F20	F61 ³	3.568(3)
F20	C24 ⁴	3.424(3)	F20	C38 ⁴	3.291(3)
F20	C54	3.568(3)	F29	F13 ¹	3.426(3)
F29	F61 ⁵	3.437(4)	F29	C25 ⁴	3.379(3)
F42	F13	3.521(3)	F42	F46 ²	3.345(3)
F42	C22 ²	3.415(3)	F42	C51 ⁶	3.399(3)
F42	C54	3.542(3)	F42	C58 ⁶	3.531(3)
F46	F42 ²	3.345(3)	F46	F61 ⁵	3.483(3)
F46	C51 ⁵	3.465(3)	F46	C54 ²	3.568(3)
F61	F20 ³	3.568(3)	F61	F29 ⁷	3.437(4)
F61	F46 ⁷	3.483(3)	F61	C24 ⁶	3.407(3)
O2	C14 ⁸	3.231(3)	O3	C7 ⁹	3.515(3)
O3	C15	3.567(3)	O3	C33 ⁹	3.073(3)
O3	C34	3.317(3)	O8	C14 ¹⁰	3.588(3)
O8	C19 ¹⁰	3.287(3)	O8	C28 ¹⁰	3.596(3)
O9	C7 ¹¹	3.286(3)	O9	C26 ¹²	3.483(3)
O9	C37 ⁷	3.545(3)	O9	C55 ⁷	3.538(3)
C7	O3 ⁹	3.515(3)	C7	O9 ¹¹	3.286(3)
C7	C14 ¹⁰	3.572(4)	C7	C19 ¹⁰	3.591(3)
C10	C11	3.597(3)	C10	C45 ¹⁰	3.595(3)
C11	C10	3.597(3)	C14	O2 ⁸	3.231(3)
C14	O8 ¹⁰	3.588(3)	C14	C7 ¹⁰	3.572(4)
C15	O3	3.567(3)	C19	O8 ¹⁰	3.287(3)
C19	C7 ¹⁰	3.591(3)	C19	C32	3.554(3)
C22	F13 ²	3.483(3)	C22	F42 ²	3.415(3)
C24	F20 ¹³	3.424(3)	C24	F61 ⁶	3.407(3)
C25	F29 ¹³	3.379(3)	C26	O9 ¹⁴	3.483(3)
C28	O8 ¹⁰	3.596(3)	C30	C39	3.312(3)
C32	C19	3.554(3)	C33	O3 ⁹	3.073(3)
C33	C43 ¹⁰	3.538(3)	C34	O3	3.317(3)
C37	O9 ⁵	3.545(3)	C38	F20 ¹³	3.291(3)

C39	C30	3.312(3)	C43	C33 ¹⁰	3.538(3)
C45	C10 ¹⁰	3.595(3)	C51	F42 ⁶	3.399(3)
C51	F46 ⁷	3.465(3)	C54	F20	3.568(3)
C54	F42	3.542(3)	C54	F46 ²	3.568(3)

Table 12. Intermolecular contacts less than 3.60 Å (continued)

atom	atom	distance	atom	atom	distance
C55	O9 ⁵	3.538(3)	C57	C58 ⁵	3.467(3)
C58	F42 ⁶	3.531(3)	C58	C57 ⁷	3.467(3)

Symmetry Operators:

(1) -X,-Y,-Z+1	(2) -X+1,-Y,-Z+1
(3) -X,-Y+1,-Z+1	(4) X-1,Y,Z
(5) X,Y-1,Z	(6) -X+1,-Y+1,-Z+1
(7) X,Y+1,Z	(8) -X+1,-Y-1,-Z+2
(9) -X,-Y,-Z+2	(10) -X+1,-Y,-Z+2
(11) -X,-Y+1,-Z+2	(12) X-1,Y+1,Z
(13) X+1,Y,Z	(14) X+1,Y-1,Z

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
F13	H22 ¹	2.759	F13	H38 ²	3.294
F13	H38 ¹	3.468	F13	H54 ¹	3.469
F20	H22 ¹	2.850	F20	H24 ²	2.922
F20	H38 ²	2.678	F20	H54	3.328
F29	H22 ²	3.466	F29	H23 ²	3.550
F29	H25 ²	2.841	F29	H38 ²	3.296
F29	H38 ¹	3.097	F42	H22 ¹	2.644
F42	H51 ³	2.724	F42	H54	2.834
F42	H58 ³	2.990	F46	H39 ¹	3.098
F46	H51 ⁴	2.761	F46	H54 ¹	2.888
F61	H22 ¹	3.335	F61	H24 ³	2.616
F61	H25 ⁵	2.998	O2	H4 ⁶	3.049
O2	H14 ⁷	2.570	O2	H28 ⁷	3.434
O3	H7A ⁶	2.897	O3	H7C ⁶	3.231
O3	H33A ⁶	3.186	O3	H33B ⁶	3.202
O3	H33C ⁶	2.386	O3	H34	2.418
O8	H1	2.891	O8	H14 ⁸	3.158
O8	H19 ⁸	2.532	O8	H28 ⁸	3.545
O8	H31 ⁸	3.306	O8	H33A	3.270
O9	H7A ⁹	3.554	O9	H7B ⁹	2.422
O9	H7C ⁹	3.515	O9	H14 ⁵	3.377
O9	H26 ⁵	2.728	O9	H37 ¹⁰	2.663
O9	H55 ¹⁰	3.189	N18	H7A ⁶	3.158
N18	H7C ⁶	3.518	N18	H34	3.148
N44	H26 ⁵	3.385	N44	H37 ¹⁰	3.317
N44	H55 ¹⁰	3.026	C1	H7A ⁶	3.538
C1	H12 ⁶	3.284	C1	H41 ⁸	3.221
C4	H11	3.377	C4	H16 ¹⁰	3.197
C4	H33C ⁶	2.979	C5	H17 ⁴	3.128
C5	H19	3.508	C5	H23	3.162
C5	H47 ⁴	3.082	C5	H58 ⁴	3.101
C6	H7A ⁶	3.224	C6	H10 ⁸	3.046
C7	H1	3.239	C7	H14 ⁸	3.177

C7	H19 ⁸	3.065	C7	H33A	3.303
C7	H37 ⁶	3.216	C10	H1	3.543
C10	H11	3.193	C10	H16 ¹⁰	3.435
C10	H28 ⁸	3.469	C10	H41 ⁸	3.524

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C11	H7A ⁶	2.861	C11	H10 ⁸	3.480
C11	H12 ⁶	3.496	C11	H41 ⁸	3.266
C12	H11	3.363	C12	H16 ¹⁰	3.304
C14	H7B ⁸	3.104	C14	H7C ⁸	3.524
C14	H17 ⁴	3.364	C14	H19	3.529
C14	H23	3.440	C14	H33B ⁷	3.007
C15	H55 ¹⁰	3.020	C16	H12 ⁶	3.320
C16	H41 ⁸	3.252	C16	H55 ⁷	3.581
C17	H33A ⁸	3.404	C17	H33B ⁸	3.354
C19	H7C ⁸	2.954	C19	H32	2.657
C19	H33A ⁸	3.094	C21	H10 ⁸	3.340
C21	H19	3.210	C21	H47 ⁴	3.195
C22	H17 ⁴	3.288	C22	H23	3.044
C22	H24 ⁴	3.404	C22	H58 ⁴	3.551
C23	H7C ⁸	3.095	C23	H32	3.585
C24	H30 ¹¹	3.308	C25	H17 ⁴	3.482
C25	H23	3.145	C25	H24 ⁴	3.231
C25	H57 ¹¹	2.780	C26	H7B ⁸	3.543
C26	H17 ⁴	3.515	C26	H23	3.318
C26	H33B ⁷	2.929	C26	H57 ¹¹	2.957
C27	H32	3.463	C28	H10 ⁸	3.526
C28	H19	3.168	C28	H47 ⁴	2.728
C30	H25 ⁵	3.292	C30	H26 ⁵	3.208
C30	H39	3.211	C31	H32	2.814
C31	H33A ⁸	3.102	C32	H19	3.180
C32	H34	3.446	C33	H4 ⁶	3.201
C33	H14 ⁷	3.174	C33	H26 ⁷	3.527
C33	H34 ⁶	3.414	C34	H26 ⁵	2.934
C34	H32	3.559	C34	H33B ⁶	3.414
C34	H39	3.368	C35	H17 ⁴	3.190
C35	H19	3.091	C35	H23	3.379
C35	H47 ⁴	2.913	C36	H30	3.563
C37	H7C ⁶	3.288	C37	H47 ⁴	3.559

C37	H58 ⁴	3.421	C38	H30 ¹¹	3.199
C39	H30	3.188	C41	H10 ⁸	3.463
C41	H11	3.226	C41	H16 ¹⁰	3.370
C43	H32	2.845	C43	H33A ⁸	2.868

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C43	H33B ⁸	3.481	C45	H7A ⁶	2.971
C45	H10 ⁸	3.040	C45	H41 ⁸	3.326
C47	H37 ¹⁰	3.526	C48	H25 ⁵	3.092
C49	H26 ⁵	3.297	C50	H1	3.071
C50	H11	3.255	C50	H14 ⁸	3.578
C50	H16 ¹⁰	3.429	C50	H28 ⁸	3.571
C51	H25 ⁵	3.537	C51	H51 ³	3.234
C51	H57 ¹⁰	3.483	C52	H38 ²	3.446
C53	H11	3.318	C53	H16 ¹⁰	3.261
C53	H33C ⁶	3.538	C53	H55 ¹⁰	3.172
C54	H30	3.337	C54	H54 ¹	3.164
C55	H10 ⁸	3.541	C55	H12 ⁶	3.546
C55	H16 ⁷	3.514	C55	H41 ⁸	3.315
C56	H22 ¹	3.182	C56	H25 ⁵	3.388
C56	H51 ³	3.590	C56	H54	3.446
C57	H23 ²	3.184	C57	H25 ²	3.458
C57	H58 ⁴	3.328	C58	H5 ¹⁰	3.600
C58	H57 ¹⁰	3.367	C59	H4 ⁶	3.402
C59	H12 ⁶	3.170	C59	H41 ⁸	3.220
C60	H38 ²	3.492	C60	H54 ¹	3.522
H1	O8	2.891	H1	C7	3.239
H1	C10	3.543	H1	C50	3.071
H1	H7A	2.741	H1	H11 ⁶	3.221
H1	H31 ⁸	3.544	H4	O2 ⁶	3.049
H4	C33 ⁶	3.201	H4	C59 ⁶	3.402
H4	H7B ⁹	3.415	H4	H12 ⁹	3.042
H4	H33B ⁶	3.460	H4	H33C ⁶	2.648
H5	C58 ⁴	3.600	H5	H17 ⁴	3.524
H5	H47 ⁴	2.976	H5	H58 ⁴	2.697
H7A	O3 ⁶	2.897	H7A	O9 ⁹	3.554
H7A	N18 ⁶	3.158	H7A	C1 ⁶	3.538
H7A	C6 ⁶	3.224	H7A	C11 ⁶	2.861
H7A	C45 ⁶	2.971	H7A	H1	2.741

H7A	H11 ⁶	2.889	H7A	H33A	3.133
H7A	H33C	3.393	H7A	H37 ⁶	3.406
H7B	O9 ⁹	2.422	H7B	C14 ⁸	3.104
H7B	C26 ⁸	3.543	H7B	H4 ⁹	3.415

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H7B	H14 ⁸	2.581	H7B	H26 ⁸	3.383
H7B	H37 ⁶	3.025	H7C	O3 ⁶	3.231
H7C	O9 ⁹	3.515	H7C	N18 ⁶	3.518
H7C	C14 ⁸	3.524	H7C	C19 ⁸	2.954
H7C	C23 ⁸	3.095	H7C	C37 ⁶	3.288
H7C	H14 ⁸	3.386	H7C	H19 ⁸	2.629
H7C	H23 ⁸	2.905	H7C	H33A	3.010
H7C	H37 ⁶	2.720	H10	C6 ⁸	3.046
H10	C11 ⁸	3.480	H10	C21 ⁸	3.340
H10	C28 ⁸	3.526	H10	C41 ⁸	3.463
H10	C45 ⁸	3.040	H10	C55 ⁸	3.541
H10	H10 ⁸	3.585	H10	H19 ⁸	3.569
H10	H28 ⁸	3.319	H10	H31 ⁸	2.860
H10	H41 ⁸	2.931	H11	C4	3.377
H11	C10	3.193	H11	C12	3.363
H11	C41	3.226	H11	C50	3.255
H11	C53	3.318	H11	H1 ⁶	3.221
H11	H7A ⁶	2.889	H11	H33C ⁶	3.109
H12	C1 ⁶	3.284	H12	C11 ⁶	3.496
H12	C16 ⁶	3.320	H12	C55 ⁶	3.546
H12	C59 ⁶	3.170	H12	H4 ⁹	3.042
H14	O2 ⁷	2.570	H14	O8 ⁸	3.158
H14	O9 ¹²	3.377	H14	C7 ⁸	3.177
H14	C33 ⁷	3.174	H14	C50 ⁸	3.578
H14	H7B ⁸	2.581	H14	H7C ⁸	3.386
H14	H16 ⁷	3.482	H14	H33B ⁷	2.774
H16	C4 ⁴	3.197	H16	C10 ⁴	3.435
H16	C12 ⁴	3.304	H16	C41 ⁴	3.370
H16	C50 ⁴	3.429	H16	C53 ⁴	3.261
H16	C55 ⁷	3.514	H16	H14 ⁷	3.482
H16	H28 ⁷	2.862	H16	H55 ⁷	3.001
H17	C5 ¹⁰	3.128	H17	C14 ¹⁰	3.364
H17	C22 ¹⁰	3.288	H17	C25 ¹⁰	3.482

H17	C26 ¹⁰	3.515	H17	C35 ¹⁰	3.190
H17	H5 ¹⁰	3.524	H17	H33B ⁸	3.472
H19	O8 ⁸	2.532	H19	C5	3.508
H19	C7 ⁸	3.065	H19	C14	3.529

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H19	C21	3.210	H19	C28	3.168
H19	C32	3.180	H19	C35	3.091
H19	H7C ⁸	2.629	H19	H10 ⁸	3.569
H19	H32	2.436	H19	H33A ⁸	3.255
H22	F13 ¹	2.759	H22	F20 ¹	2.850
H22	F29 ¹¹	3.466	H22	F42 ¹	2.644
H22	F61 ¹	3.335	H22	C56 ¹	3.182
H22	H23	3.449	H22	H24 ⁴	3.497
H22	H58 ⁴	3.511	H23	F29 ¹¹	3.550
H23	C5	3.162	H23	C14	3.440
H23	C22	3.044	H23	C25	3.145
H23	C26	3.318	H23	C35	3.379
H23	C57 ¹¹	3.184	H23	H7C ⁸	2.905
H23	H22	3.449	H23	H57 ¹¹	2.813
H24	F20 ¹¹	2.922	H24	F61 ³	2.616
H24	C22 ¹⁰	3.404	H24	C25 ¹⁰	3.231
H24	H22 ¹⁰	3.497	H24	H25 ¹⁰	3.200
H24	H30 ¹¹	3.252	H25	F29 ¹¹	2.841
H25	F61 ¹²	2.998	H25	C30 ¹²	3.292
H25	C48 ¹²	3.092	H25	C51 ¹²	3.537
H25	C56 ¹²	3.388	H25	C57 ¹¹	3.458
H25	H24 ⁴	3.200	H25	H30 ¹²	3.518
H25	H57 ¹¹	2.533	H26	O9 ¹²	2.728
H26	N44 ¹²	3.385	H26	C30 ¹²	3.208
H26	C33 ⁷	3.527	H26	C34 ¹²	2.934
H26	C49 ¹²	3.297	H26	H7B ⁸	3.383
H26	H30 ¹²	3.501	H26	H33B ⁷	2.647
H26	H34 ¹²	3.077	H26	H37 ¹¹	3.397
H26	H57 ¹¹	2.827	H28	O2 ⁷	3.434
H28	O8 ⁸	3.545	H28	C10 ⁸	3.469
H28	C50 ⁸	3.571	H28	H10 ⁸	3.319
H28	H16 ⁷	2.862	H28	H47 ⁴	2.899
H30	C24 ²	3.308	H30	C36	3.563

H30	C38 ²	3.199	H30	C39	3.188
H30	C54	3.337	H30	H24 ²	3.252
H30	H25 ⁵	3.518	H30	H26 ⁵	3.501
H30	H33B ⁶	3.482	H30	H38 ²	3.087

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H30	H39	3.363	H31	O8 ^s	3.306
H31	H1 ^s	3.544	H31	H10 ^s	2.860
H31	H32	2.911	H31	H33A ^s	2.964
H32	C19	2.657	H32	C23	3.585
H32	C27	3.463	H32	C31	2.814
H32	C34	3.559	H32	C43	2.845
H32	H19	2.436	H32	H31	2.911
H32	H34	3.246	H33A	O3 ⁶	3.186
H33A	O8	3.270	H33A	C7	3.303
H33A	C17 ^s	3.404	H33A	C19 ^s	3.094
H33A	C31 ^s	3.102	H33A	C43 ^s	2.868
H33A	H7A	3.133	H33A	H7C	3.010
H33A	H19 ^s	3.255	H33A	H31 ^s	2.964
H33B	O3 ⁶	3.202	H33B	C14 ⁷	3.007
H33B	C17 ^s	3.354	H33B	C26 ⁷	2.929
H33B	C34 ⁶	3.414	H33B	C43 ^s	3.481
H33B	H4 ⁶	3.460	H33B	H14 ⁷	2.774
H33B	H17 ^s	3.472	H33B	H26 ⁷	2.647
H33B	H30 ⁶	3.482	H33B	H34 ⁶	2.847
H33C	O3 ⁶	2.386	H33C	C4 ⁶	2.979
H33C	C53 ⁶	3.538	H33C	H4 ⁶	2.648
H33C	H7A	3.393	H33C	H11 ⁶	3.109
H33C	H34 ⁶	3.111	H34	O3	2.418
H34	N18	3.148	H34	C32	3.446
H34	C33 ⁶	3.414	H34	H26 ⁵	3.077
H34	H32	3.246	H34	H33B ⁶	2.847
H34	H33C ⁶	3.111	H37	O9 ⁴	2.663
H37	N44 ⁴	3.317	H37	C7 ⁶	3.216
H37	C47 ⁴	3.526	H37	H7A ⁶	3.406
H37	H7B ⁶	3.025	H37	H7C ⁶	2.720
H37	H26 ²	3.397	H37	H47 ⁴	3.240
H38	F13 ¹¹	3.294	H38	F13 ¹	3.468
H38	F20 ¹¹	2.678	H38	F29 ¹¹	3.296

H38	F29 ¹	3.097	H38	C52 ¹¹	3.446
H38	C60 ¹¹	3.492	H38	H30 ¹¹	3.087
H39	F46 ¹	3.098	H39	C30	3.211
H39	C34	3.368	H39	H30	3.363

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H41	C1 ⁸	3.221	H41	C10 ⁸	3.524
H41	C11 ⁸	3.266	H41	C16 ⁸	3.252
H41	C45 ⁸	3.326	H41	C55 ⁸	3.315
H41	C59 ⁸	3.220	H41	H10 ⁸	2.931
H47	C5 ¹⁰	3.082	H47	C21 ¹⁰	3.195
H47	C28 ¹⁰	2.728	H47	C35 ¹⁰	2.913
H47	C37 ¹⁰	3.559	H47	H5 ¹⁰	2.976
H47	H28 ¹⁰	2.899	H47	H37 ¹⁰	3.240
H51	F42 ³	2.724	H51	F46 ¹⁰	2.761
H51	C51 ³	3.234	H51	C56 ³	3.590
H51	H51 ³	2.569	H54	F13 ¹	3.469
H54	F20	3.328	H54	F42	2.834
H54	F46 ¹	2.888	H54	C54 ¹	3.164
H54	C56	3.446	H54	C60 ¹	3.522
H54	H54 ¹	2.535	H55	O9 ⁴	3.189
H55	N44 ⁴	3.026	H55	C15 ⁴	3.020
H55	C16 ⁷	3.581	H55	C53 ⁴	3.172
H55	H16 ⁷	3.001	H57	C25 ²	2.780
H57	C26 ²	2.957	H57	C51 ⁴	3.483
H57	C58 ⁴	3.367	H57	H23 ²	2.813
H57	H25 ²	2.533	H57	H26 ²	2.827
H57	H58 ⁴	3.492	H58	F42 ³	2.990
H58	C5 ¹⁰	3.101	H58	C22 ¹⁰	3.551
H58	C37 ¹⁰	3.421	H58	C57 ¹⁰	3.328
H58	H5 ¹⁰	2.697	H58	H22 ¹⁰	3.511
H58	H57 ¹⁰	3.492			

Symmetry Operators:

(1) -X+1,-Y,-Z+1	(2) X-1,Y,Z
(3) -X+1,-Y+1,-Z+1	(4) X,Y-1,Z
(5) X-1,Y+1,Z	(6) -X,-Y,-Z+2

$$(7) \quad -X+1, -Y-1, -Z+2$$

$$(9) \quad -X, -Y+1, -Z+2$$

$$(11) \quad X+1, Y, Z$$

$$(8) \quad -X+1, -Y, -Z+2$$

$$(10) \quad X, Y+1, Z$$

$$(12) \quad X+1, Y-1, Z$$

Computational details.

Geometries of **A** and **B** were optimized using density functional theory (DFT),¹ which utilized Becke's three-parameter exchange-correlation functionals² including the nonlocal gradient corrections described by Lee-Yang-Parr (LYP),³ as implemented in the Gaussian 03 program package.⁴ All geometry optimizations were performed using 6-311++G(2d, p) basis set. Initial geometry was taken from crystal structure. NMR chemical shifts were computed with the gauge-invariant atomic orbital (GIAO) approach⁵ in conjunction with the B3LYP functional.^{2,3} The absolute shifts (σ) of tetramethylsilane (TMS) for ^1H and ^{13}C and ammonia (NH_3) for ^{14}N were used to compute the relative chemical shifts $\delta^\dagger = \sigma_{\text{reference}} - \sigma_{\text{compound}}$.

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Cyclic nitrone **A**

E(RB + HF – BLYP) = –1430.45826085 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	9	0	-4.935496	-2.551529	-2.113511
2	9	0	-6.080524	-1.531625	-0.578835
3	9	0	-5.271214	-3.503597	-0.190141
4	8	0	7.080362	-0.850580	-0.990335
5	8	0	1.098230	-1.987726	1.903127
6	7	0	0.983843	-0.864611	1.369738
7	6	0	3.789346	-1.487633	0.541445
8	6	0	7.783137	-2.055239	-0.709337
9	6	0	5.160201	0.475517	-0.868799
10	6	0	5.102118	-1.712878	0.149173
11	6	0	1.770811	-0.058559	0.649169
12	6	0	-1.585753	3.040842	0.775055
13	6	0	-0.289838	4.315360	-0.796013
14	6	0	-1.285408	5.281065	-0.843048
15	6	0	-2.580718	4.006597	0.728154
16	6	0	0.747070	0.980667	0.551288
17	6	0	-2.830297	-1.086832	-1.104970
18	6	0	0.679429	2.201909	-0.000509
19	6	0	-1.689444	-0.488293	-0.586804
20	6	0	-2.439487	5.130850	-0.081343
21	6	0	3.855608	0.694242	-0.477241
22	6	0	-0.416725	3.169794	0.007334
23	6	0	-0.198249	0.096396	1.373545
24	6	0	-3.740867	-1.698899	-0.249873
25	6	0	-1.450348	-0.488353	0.786741
26	6	0	5.796971	-0.731671	-0.559910
27	6	0	-3.512012	-1.707853	1.123737
28	6	0	3.137401	-0.282470	0.237082
29	6	0	-4.998723	-2.322262	-0.786700
30	6	0	-2.373904	-1.102871	1.635301
31	1	0	3.255623	-2.249826	1.092038
32	1	0	7.291688	-2.917632	-1.168530
33	1	0	7.877287	-2.217560	0.368145
34	1	0	8.772198	-1.929058	-1.143675
35	1	0	5.712103	1.228023	-1.417670
36	1	0	5.569768	-2.653816	0.402385
37	1	0	-1.723111	2.185005	1.420712

38	1	0	0.606267	4.442506	-1.393620
39	1	0	-1.159518	6.152383	-1.474846
40	1	0	-3.472802	3.882599	1.330718
41	1	0	-3.009860	-1.080357	-2.171531
42	1	0	1.554508	2.537368	-0.545630
43	1	0	-0.984217	-0.012120	-1.255906
44	1	0	-3.219015	5.882275	-0.113519
45	1	0	3.390768	1.637622	-0.726531
46	1	0	-0.363241	0.443913	2.396318
47	1	0	-4.216907	-2.190598	1.788420
48	1	0	-2.193963	-1.117800	2.703743

β -lactam **B**

E(RB + HF – BLYP) = -1430.53016119 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	9	0	-5.064156	-2.484067	-2.022604
2	9	0	-6.090678	-0.911444	-0.940416
3	9	0	-5.828912	-2.858885	-0.023725
4	8	0	7.087322	-0.745217	-0.816665
5	8	0	1.091098	-2.282677	1.890713
6	7	0	1.768842	-0.302681	0.767290
7	6	0	3.581872	-1.652943	-0.110954
8	6	0	7.625598	-1.972323	-1.291663
9	6	0	5.306732	0.520296	0.017537
10	6	0	4.908407	-1.801314	-0.502419
11	6	0	-1.312701	2.994516	0.808363
12	6	0	0.938352	-1.169329	1.475573
13	6	0	-0.008059	3.984474	-0.948669
14	6	0	-0.943239	5.002683	-1.075862
15	6	0	-2.246920	4.013020	0.681277
16	6	0	0.797131	0.729663	0.679610

17	6	0	-2.922283	-0.965002	-1.047975
18	6	0	0.854506	1.913499	0.063579
19	6	0	-1.730172	-0.502245	-0.509558
20	6	0	-2.071131	5.021501	-0.262270
21	6	0	3.991242	0.661009	0.419313
22	6	0	-0.174112	2.952876	-0.011201
23	6	0	-0.203017	-0.107167	1.477823
24	6	0	-3.909091	-1.482141	-0.213347
25	6	0	-1.507792	-0.543510	0.867717
26	6	0	5.777251	-0.711288	-0.447648
27	6	0	-3.700370	-1.529154	1.161385
28	6	0	3.114143	-0.425703	0.348098
29	6	0	-5.215811	-1.938110	-0.796657
30	6	0	-2.507059	-1.061399	1.693812
31	1	0	2.911554	-2.500983	-0.150141
32	1	0	7.112314	-2.307228	-2.197880
33	1	0	7.568298	-2.753867	-0.528328
34	1	0	8.668915	-1.769096	-1.522216
35	1	0	5.994586	1.354812	0.067353
36	1	0	5.245524	-2.767503	-0.849429
37	1	0	-1.469593	2.233141	1.560141
38	1	0	0.867974	3.979726	-1.588109
39	1	0	-0.789704	5.783836	-1.811160
40	1	0	-3.117479	4.021496	1.326630
41	1	0	-3.083490	-0.927046	-2.117492
42	1	0	1.768509	2.132551	-0.478848
43	1	0	-0.971231	-0.094829	-1.165361
44	1	0	-2.802471	5.814902	-0.357270
45	1	0	3.647213	1.611720	0.804473
46	1	0	-0.355484	0.269760	2.492361
47	1	0	-4.463903	-1.933802	1.812465
48	1	0	-2.347929	-1.107563	2.764925