APPENDIX 2

X-Ray Crystallography Reports Relevant to Chapter 2:

Development of a Diastereoselective 1,2-Addition to Sulfinyl Imines[†]

[†] The work disclosed in this appendix for the X-ray crystallographic analysis of **97d** was completed entirely by Larry Henling and Dr. Michael Day in the Caltech X-ray crystallography lab.

A2.1 Crystal Structure analysis of sulfinamide 97d

Figure A2.1. Sulfinamide **97d**. Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 780836.

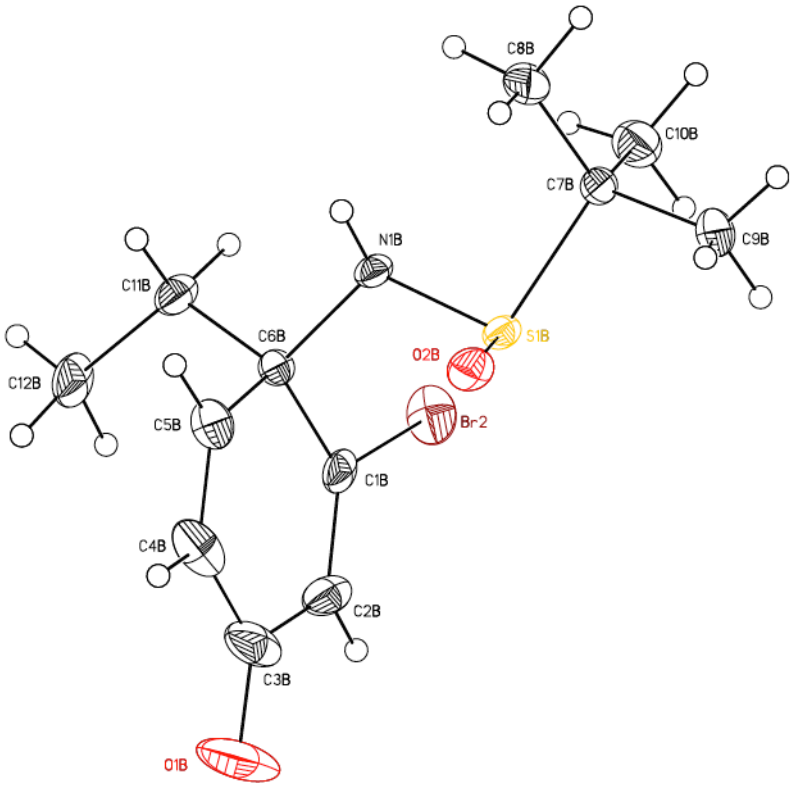
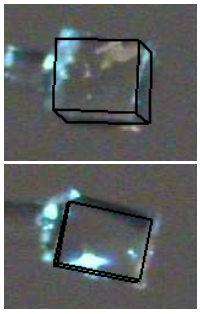


Table A2.1. Crystal data and structure refinement for sulfinamide **97d** (CCDC 780836).



Empirical formula	$C_{12}H_{18}BrNO_2S$
Formula weight	320.24
Crystallization Solvent	Benzene
Crystal Habit	Block
Crystal size	0.19 x 0.17 x 0.15 mm^3
Crystal color	Pale yellow

Data Collection

Type of diffractometer	Bruker KAPPA APEX II	
Wavelength	0.71073 Å MoKα	
Data Collection Temperature	100(2) K	
θ range for 9971 reflections used in lattice determination	2.36 to 28.59°	
Unit cell dimensions	a = 9.9624(4) Å b = 17.8137(8) Å c = 12.6175(6) Å	α= 90° β= 98.264(2)° γ = 90°
Volume	2215.94(17) $Å^3$	
Z	6	
Crystal system	Monoclinic	
Space group	$P2_1$	
Density (calculated)	1.440 Mg/m^3	
F(000)	984	
Data collection program	Bruker APEX2 v2009.7-0	
θ range for data collection	1.63 to 29.93°	
Completeness to θ = 29.93°	99.9 %	
Index ranges	$-13 \leq h \leq 13$, $-25 \leq k \leq 25$, $-17 \leq l \leq 17$	
Data collection scan type	ω scans; 9 settings	
Data reduction program	Bruker SAINT-Plus v7.66A	
Reflections collected	50720	
Independent reflections	12745 [R_{int}= 0.0422]	
Absorption coefficient	2.915 mm^{-1}	
Absorption correction	Gaussian	
Max. and min. transmission	0.7274 and 0.6375	

Table A2.1.(continued)

Structure solution and Refinement

Structure solution program	Bruker XS 2008/1
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	Bruker XL 2008/1
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	12745 / 1 / 676
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.083
Final R indices [$I>2\sigma(I)$, 10731 reflections]	R1 = 0.0257, *w*R2 = 0.0308
R indices (all data)	R1 = 0.0344, *w*R2 = 0.0315
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.003
Average shift/error	0.000
Absolute structure determination	Anomalous differences
Absolute structure parameter	-0.011(2)
Largest diff. peak and hole	0.896 and -0.565 e.$Å^{-3}$

Special Refinement Details

Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table A2.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for RUN02 (CCDC 780836). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Br(1)	826(1)	7627(1)	10809(1)	30(1)
S(1A)	290(1)	9531(1)	9058(1)	15(1)
O(1A)	4648(1)	8151(1)	8555(1)	29(1)
O(2A)	793(1)	10261(1)	8672(1)	20(1)
N(1A)	792(2)	9400(1)	10355(1)	16(1)
C(1A)	2103(2)	8250(1)	10247(2)	18(1)
C(2A)	2902(2)	7960(1)	9602(2)	21(1)
C(3A)	3913(2)	8416(1)	9154(2)	21(1)
C(4A)	3986(2)	9211(1)	9477(2)	21(1)
C(5A)	3198(2)	9493(1)	10137(2)	18(1)
C(6A)	2156(2)	9055(1)	10635(2)	15(1)
C(7A)	-1532(2)	9678(1)	9070(2)	17(1)
C(8A)	-1753(2)	10415(1)	9636(2)	22(1)
C(9A)	-2121(2)	9721(2)	7891(2)	31(1)
C(10A)	-2076(2)	9004(1)	9603(2)	28(1)
C(11A)	2518(2)	9089(1)	11865(2)	22(1)
C(12A)	3829(2)	8682(1)	12286(2)	27(1)
Br(2)	5571(1)	1465(1)	7107(1)	31(1)
S(1B)	2422(1)	501(1)	5939(1)	16(1)
O(1B)	1957(2)	3439(1)	5749(1)	58(1)
O(2B)	965(1)	639(1)	5519(1)	22(1)
N(1B)	2730(2)	670(1)	7254(1)	16(1)
C(1B)	3798(2)	1872(1)	6934(2)	19(1)
C(2B)	3526(2)	2495(1)	6370(2)	27(1)
C(3B)	2179(2)	2846(1)	6243(2)	36(1)
C(4B)	1137(2)	2458(1)	6737(2)	33(1)
C(5B)	1425(2)	1837(1)	7295(2)	24(1)
C(6B)	2796(2)	1481(1)	7539(1)	16(1)
C(7B)	2599(2)	-528(1)	5961(2)	19(1)
C(8B)	1628(2)	-877(1)	6636(2)	26(1)
C(9B)	2225(3)	-737(1)	4781(2)	35(1)
C(10B)	4062(2)	-713(1)	6359(2)	29(1)
C(11B)	3279(2)	1518(1)	8758(2)	21(1)
C(12B)	3509(2)	2312(1)	9194(2)	28(1)
Br(3)	2741(1)	7173(1)	5606(1)	35(1)
S(1C)	64(1)	6168(1)	7644(1)	17(1)
O(1C)	4996(2)	5914(1)	9071(1)	52(1)
O(2C)	-642(1)	5473(1)	7941(1)	22(1)
N(1C)	570(2)	6064(1)	6458(1)	17(1)
C(1C)	2956(2)	6399(1)	6656(1)	20(1)
C(2C)	3922(2)	6447(1)	7474(2)	25(1)
C(3C)	4149(2)	5852(1)	8278(2)	28(1)
C(4C)	3287(2)	5189(1)	8077(2)	25(1)
C(5C)	2288(2)	5153(1)	7278(2)	23(1)

C(6C)	1962(2)	5764(1)	6444(2)	17(1)
C(7C)	-1303(2)	6864(1)	7301(2)	19(1)
C(8C)	-2331(2)	6590(1)	6379(2)	26(1)
C(9C)	-1951(2)	6934(1)	8319(2)	28(1)
C(10C)	-630(2)	7594(1)	7045(2)	33(1)
C(11C)	1989(2)	5403(1)	5324(2)	26(1)
C(12C)	3403(2)	5133(2)	5166(2)	32(1)

Table A2.3. Bond lengths [Å] and angles [°] for RUN02 (CCDC 780836).

Br(1)-C(1A)	1.9001(18)	C(6B)-C(11B)	1.546(2)
S(1A)-O(2A)	1.4999(13)	C(7B)-C(10B)	1.508(3)
S(1A)-N(1A)	1.6576(17)	C(7B)-C(8B)	1.512(3)
S(1A)-C(7A)	1.8365(16)	C(7B)-C(9B)	1.528(3)
O(1A)-C(3A)	1.220(2)	C(8B)-H(8B1)	0.920(18)
N(1A)-C(6A)	1.486(2)	C(8B)-H(8B2)	0.917(17)
N(1A)-H(1A)	0.692(16)	C(8B)-H(8B3)	1.001(19)
C(1A)-C(2A)	1.323(3)	C(9B)-H(9B1)	0.965(19)
C(1A)-C(6A)	1.515(2)	C(9B)-H(9B2)	0.93(2)
C(2A)-C(3A)	1.469(3)	C(9B)-H(9B3)	0.872(19)
C(2A)-H(2A)	0.928(17)	C(10B)-H(10D)	0.902(19)
C(3A)-C(4A)	1.474(3)	C(10B)-H(10E)	0.94(2)
C(4A)-C(5A)	1.323(3)	C(10B)-H(10F)	0.96(2)
C(4A)-H(4A)	0.935(19)	C(11B)-C(12B)	1.523(3)
C(5A)-C(6A)	1.506(2)	C(11B)-H(11C)	0.871(18)
C(5A)-H(5A)	0.950(16)	C(11B)-H(11D)	1.093(17)
C(6A)-C(11A)	1.542(3)	C(12B)-H(12D)	1.02(2)
C(7A)-C(8A)	1.526(3)	C(12B)-H(12E)	0.889(16)
C(7A)-C(10A)	1.514(3)	C(12B)-H(12F)	0.99(2)
C(7A)-C(9A)	1.521(3)	Br(3)-C(1C)	1.9030(18)
C(8A)-H(8A1)	0.89(2)	S(1C)-O(2C)	1.4983(12)
C(8A)-H(8A2)	0.998(18)	S(1C)-N(1C)	1.6569(16)
C(8A)-H(8A3)	0.980(18)	S(1C)-C(7C)	1.8452(18)
C(9A)-H(9A1)	0.93(2)	O(1C)-C(3C)	1.218(2)
C(9A)-H(9A2)	0.95(2)	N(1C)-C(6C)	1.489(2)
C(9A)-H(9A3)	0.923(19)	N(1C)-H(1C)	0.876(17)
C(10A)-H(10A)	0.963(17)	C(1C)-C(2C)	1.308(2)
C(10A)-H(10B)	1.01(2)	C(1C)-C(6C)	1.503(2)
C(10A)-H(10C)	0.879(18)	C(2C)-C(3C)	1.462(3)
C(11A)-C(12A)	1.522(3)	C(2C)-H(2C)	0.777(17)
C(11A)-H(11A)	0.959(16)	C(3C)-C(4C)	1.461(3)
C(11A)-H(11B)	0.947(18)	C(4C)-C(5C)	1.313(3)
C(12A)-H(12A)	0.989(16)	C(4C)-H(4C)	0.864(17)
C(12A)-H(12B)	0.877(18)	C(5C)-C(6C)	1.516(3)
C(12A)-H(12C)	0.94(2)	C(5C)-H(5C)	0.901(17)
Br(2)-C(1B)	1.8929(18)	C(6C)-C(11C)	1.557(3)
S(1B)-O(2B)	1.4923(12)	C(7C)-C(10C)	1.519(3)
S(1B)-N(1B)	1.6709(16)	C(7C)-C(8C)	1.516(3)
S(1B)-C(7B)	1.8405(19)	C(7C)-C(9C)	1.523(3)
O(1B)-C(3B)	1.230(2)	C(8C)-H(8C1)	0.884(18)
N(1B)-C(6B)	1.487(2)	C(8C)-H(8C2)	0.970(17)
N(1B)-H(1B)	0.802(17)	C(8C)-H(8C3)	1.001(17)
C(1B)-C(2B)	1.326(3)	C(9C)-H(9C1)	1.026(17)
C(1B)-C(6B)	1.510(2)	C(9C)-H(9C2)	0.915(19)
C(2B)-C(3B)	1.468(3)	C(9C)-H(9C3)	0.945(18)
C(2B)-H(2B)	0.850(17)	C(10C)-H(10G)	0.944(18)
C(3B)-C(4B)	1.459(3)	C(10C)-H(10H)	0.983(18)
C(4B)-C(5B)	1.321(3)	C(10C)-H(10I)	0.952(18)
C(4B)-H(4B)	0.956(17)	C(11C)-C(12C)	1.528(3)
C(5B)-C(6B)	1.498(2)	C(11C)-H(11E)	1.01(2)
C(5B)-H(5B)	0.870(18)	C(11C)-H(11F)	1.023(17)

C(12C)-H(12G)	1.008(18)	H(10B)-C(10A)-H(10C)	101.7(16)
C(12C)-H(12H)	1.10(2)	C(12A)-C(11A)-C(6A)	113.45(18)
C(12C)-H(12I)	0.93(2)	C(12A)-C(11A)-H(11A)	107.7(10)
		C(6A)-C(11A)-H(11A)	111.0(10)
O(2A)-S(1A)-N(1A)	112.07(8)	C(12A)-C(11A)-H(11B)	109.9(11)
O(2A)-S(1A)-C(7A)	104.84(8)	C(6A)-C(11A)-H(11B)	107.2(11)
N(1A)-S(1A)-C(7A)	99.80(8)	H(11A)-C(11A)-H(11B)	107.5(15)
C(6A)-N(1A)-S(1A)	115.40(13)	C(11A)-C(12A)-H(12A)	111.2(10)
C(6A)-N(1A)-H(1A)	112.6(15)	C(11A)-C(12A)-H(12B)	110.5(12)
S(1A)-N(1A)-H(1A)	117.1(15)	H(12A)-C(12A)-H(12B)	99.9(15)
C(2A)-C(1A)-C(6A)	124.94(17)	C(11A)-C(12A)-H(12C)	115.8(13)
C(2A)-C(1A)-Br(1)	119.77(15)	H(12A)-C(12A)-H(12C)	110.5(16)
C(6A)-C(1A)-Br(1)	115.23(13)	H(12B)-C(12A)-H(12C)	107.8(17)
C(1A)-C(2A)-C(3A)	121.87(19)	O(2B)-S(1B)-N(1B)	110.72(8)
C(1A)-C(2A)-H(2A)	123.4(12)	O(2B)-S(1B)-C(7B)	104.83(8)
C(3A)-C(2A)-H(2A)	114.7(11)	N(1B)-S(1B)-C(7B)	99.28(8)
O(1A)-C(3A)-C(2A)	122.06(19)	C(6B)-N(1B)-S(1B)	114.29(12)
O(1A)-C(3A)-C(4A)	122.21(18)	C(6B)-N(1B)-H(1B)	111.7(13)
C(2A)-C(3A)-C(4A)	115.73(17)	S(1B)-N(1B)-H(1B)	114.8(12)
C(5A)-C(4A)-C(3A)	121.95(19)	C(2B)-C(1B)-C(6B)	123.94(18)
C(5A)-C(4A)-H(4A)	122.4(12)	C(2B)-C(1B)-Br(2)	119.82(15)
C(3A)-C(4A)-H(4A)	115.6(12)	C(6B)-C(1B)-Br(2)	116.06(13)
C(4A)-C(5A)-C(6A)	124.99(18)	C(1B)-C(2B)-C(3B)	121.9(2)
C(4A)-C(5A)-H(5A)	122.8(11)	C(1B)-C(2B)-H(2B)	120.1(13)
C(6A)-C(5A)-H(5A)	112.2(11)	C(3B)-C(2B)-H(2B)	117.8(12)
N(1A)-C(6A)-C(5A)	110.39(15)	O(1B)-C(3B)-C(4B)	122.4(2)
N(1A)-C(6A)-C(1A)	109.04(15)	O(1B)-C(3B)-C(2B)	121.1(2)
C(5A)-C(6A)-C(1A)	110.46(15)	C(4B)-C(3B)-C(2B)	116.51(18)
N(1A)-C(6A)-C(11A)	107.28(15)	C(5B)-C(4B)-C(3B)	120.8(2)
C(5A)-C(6A)-C(11A)	108.89(15)	C(5B)-C(4B)-H(4B)	120.3(12)
C(1A)-C(6A)-C(11A)	110.74(16)	C(3B)-C(4B)-H(4B)	118.8(12)
C(8A)-C(7A)-C(10A)	112.94(18)	C(4B)-C(5B)-C(6B)	125.9(2)
C(8A)-C(7A)-C(9A)	110.65(17)	C(4B)-C(5B)-H(5B)	122.5(13)
C(10A)-C(7A)-C(9A)	111.22(18)	C(6B)-C(5B)-H(5B)	111.0(13)
C(8A)-C(7A)-S(1A)	109.64(12)	N(1B)-C(6B)-C(5B)	110.73(14)
C(10A)-C(7A)-S(1A)	107.97(13)	N(1B)-C(6B)-C(1B)	109.52(14)
C(9A)-C(7A)-S(1A)	104.01(13)	C(5B)-C(6B)-C(1B)	110.50(16)
C(7A)-C(8A)-H(8A1)	110.2(13)	N(1B)-C(6B)-C(11B)	106.15(15)
C(7A)-C(8A)-H(8A2)	111.9(10)	C(5B)-C(6B)-C(11B)	109.37(15)
H(8A1)-C(8A)-H(8A2)	106.4(16)	C(1B)-C(6B)-C(11B)	110.47(15)
C(7A)-C(8A)-H(8A3)	111.8(11)	C(10B)-C(7B)-C(8B)	112.85(18)
H(8A1)-C(8A)-H(8A3)	107.7(16)	C(10B)-C(7B)-C(9B)	111.09(19)
H(8A2)-C(8A)-H(8A3)	108.6(14)	C(8B)-C(7B)-C(9B)	111.26(18)
C(7A)-C(9A)-H(9A1)	108.1(13)	C(10B)-C(7B)-S(1B)	108.01(14)
C(7A)-C(9A)-H(9A2)	115.5(13)	C(8B)-C(7B)-S(1B)	110.51(14)
H(9A1)-C(9A)-H(9A2)	109.5(18)	C(9B)-C(7B)-S(1B)	102.61(14)
C(7A)-C(9A)-H(9A3)	112.2(12)	C(7B)-C(8B)-H(8B1)	110.1(12)
H(9A1)-C(9A)-H(9A3)	111.3(17)	C(7B)-C(8B)-H(8B2)	111.6(12)
H(9A2)-C(9A)-H(9A3)	100.1(16)	H(8B1)-C(8B)-H(8B2)	102.4(16)
C(7A)-C(10A)-H(10A)	112.4(11)	C(7B)-C(8B)-H(8B3)	112.6(11)
C(7A)-C(10A)-H(10B)	109.0(11)	H(8B1)-C(8B)-H(8B3)	108.1(16)
H(10A)-C(10A)-H(10B)	111.3(15)	H(8B2)-C(8B)-H(8B3)	111.5(16)
C(7A)-C(10A)-H(10C)	110.9(12)	C(7B)-C(9B)-H(9B1)	110.0(12)
H(10A)-C(10A)-H(10C)	111.0(17)	C(7B)-C(9B)-H(9B2)	119.6(15)

H(9B1)-C(9B)-H(9B2)	110.7(19)	N(1C)-C(6C)-C(5C)	110.89(14)
C(7B)-C(9B)-H(9B3)	115.6(13)	N(1C)-C(6C)-C(1C)	108.60(15)
H(9B1)-C(9B)-H(9B3)	98.6(16)	C(5C)-C(6C)-C(1C)	110.28(15)
H(9B2)-C(9B)-H(9B3)	100.2(18)	N(1C)-C(6C)-C(11C)	107.28(14)
C(7B)-C(10B)-H(10D)	112.5(12)	C(5C)-C(6C)-C(11C)	107.68(16)
C(7B)-C(10B)-H(10E)	111.4(13)	C(1C)-C(6C)-C(11C)	112.08(16)
H(10D)-C(10B)-H(10E)	108.8(17)	C(10C)-C(7C)-C(8C)	112.51(18)
C(7B)-C(10B)-H(10F)	108.6(12)	C(10C)-C(7C)-C(9C)	111.21(17)
H(10D)-C(10B)-H(10F)	111.5(18)	C(8C)-C(7C)-C(9C)	110.61(17)
H(10E)-C(10B)-H(10F)	103.7(17)	C(10C)-C(7C)-S(1C)	106.92(14)
C(12B)-C(11B)-C(6B)	114.06(18)	C(8C)-C(7C)-S(1C)	111.00(13)
C(12B)-C(11B)-H(11C)	106.1(13)	C(9C)-C(7C)-S(1C)	104.22(14)
C(6B)-C(11B)-H(11C)	109.5(12)	C(7C)-C(8C)-H(8C1)	107.8(12)
C(12B)-C(11B)-H(11D)	110.7(9)	C(7C)-C(8C)-H(8C2)	112.5(10)
C(6B)-C(11B)-H(11D)	106.9(9)	H(8C1)-C(8C)-H(8C2)	103.0(14)
H(11C)-C(11B)-H(11D)	109.5(15)	C(7C)-C(8C)-H(8C3)	112.1(10)
C(11B)-C(12B)-H(12D)	114.0(12)	H(8C1)-C(8C)-H(8C3)	108.1(15)
C(11B)-C(12B)-H(12E)	112.1(12)	H(8C2)-C(8C)-H(8C3)	112.7(15)
H(12D)-C(12B)-H(12E)	101.4(15)	C(7C)-C(9C)-H(9C1)	112.6(9)
C(11B)-C(12B)-H(12F)	118.9(12)	C(7C)-C(9C)-H(9C2)	112.0(12)
H(12D)-C(12B)-H(12F)	102.0(16)	H(9C1)-C(9C)-H(9C2)	112.0(14)
H(12E)-C(12B)-H(12F)	106.5(15)	C(7C)-C(9C)-H(9C3)	106.0(12)
O(2C)-S(1C)-N(1C)	110.32(8)	H(9C1)-C(9C)-H(9C3)	112.0(15)
O(2C)-S(1C)-C(7C)	104.89(8)	H(9C2)-C(9C)-H(9C3)	101.6(16)
N(1C)-S(1C)-C(7C)	100.00(8)	C(7C)-C(10C)-H(10G)	109.8(12)
C(6C)-N(1C)-S(1C)	117.11(12)	C(7C)-C(10C)-H(10H)	108.1(13)
C(6C)-N(1C)-H(1C)	116.4(11)	H(10G)-C(10C)-H(10H)	108.3(16)
S(1C)-N(1C)-H(1C)	114.4(12)	C(7C)-C(10C)-H(10I)	108.6(11)
C(2C)-C(1C)-C(6C)	125.51(18)	H(10G)-C(10C)-H(10I)	113.9(16)
C(2C)-C(1C)-Br(3)	119.91(16)	H(10H)-C(10C)-H(10I)	107.9(16)
C(6C)-C(1C)-Br(3)	114.58(13)	C(12C)-C(11C)-C(6C)	112.65(17)
C(1C)-C(2C)-C(3C)	121.5(2)	C(12C)-C(11C)-H(11E)	111.8(11)
C(1C)-C(2C)-H(2C)	120.4(15)	C(6C)-C(11C)-H(11E)	105.5(12)
C(3C)-C(2C)-H(2C)	118.1(15)	C(12C)-C(11C)-H(11F)	109.6(10)
O(1C)-C(3C)-C(2C)	121.6(2)	C(6C)-C(11C)-H(11F)	111.4(10)
O(1C)-C(3C)-C(4C)	122.4(2)	H(11E)-C(11C)-H(11F)	105.6(14)
C(2C)-C(3C)-C(4C)	115.94(18)	C(11C)-C(12C)-H(12G)	109.7(10)
C(5C)-C(4C)-C(3C)	122.3(2)	C(11C)-C(12C)-H(12H)	111.2(12)
C(5C)-C(4C)-H(4C)	121.7(13)	H(12G)-C(12C)-H(12H)	111.9(16)
C(3C)-C(4C)-H(4C)	115.8(13)	C(11C)-C(12C)-H(12I)	108.2(14)
C(4C)-C(5C)-C(6C)	124.19(19)	H(12G)-C(12C)-H(12I)	117.4(17)
C(4C)-C(5C)-H(5C)	122.4(12)	H(12H)-C(12C)-H(12I)	98.0(18)
C(6C)-C(5C)-H(5C)	113.3(12)		

Table A2.4. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for RUN02 (CCDC 780836). The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	290(1)	195(1)	416(1)	73(1)	92(1)	-18(1)
S(1A)	142(2)	172(2)	140(3)	1(2)	13(2)	9(2)
O(1A)	290(8)	349(9)	232(9)	-12(7)	76(7)	118(7)
O(2A)	210(7)	205(7)	188(7)	65(6)	55(6)	-21(6)
N(1A)	186(8)	144(9)	143(9)	-24(8)	22(7)	34(7)
C(1A)	167(9)	159(10)	208(11)	32(9)	-33(8)	11(8)
C(2A)	233(10)	153(11)	224(12)	-12(9)	0(9)	40(9)
C(3A)	195(10)	257(11)	153(11)	43(9)	-43(8)	73(8)
C(4A)	145(9)	250(12)	246(12)	42(10)	24(8)	-19(8)
C(5A)	140(8)	151(10)	219(11)	1(9)	-39(8)	16(8)
C(6A)	148(9)	148(10)	140(10)	3(8)	10(8)	37(7)
C(7A)	130(9)	161(10)	203(11)	10(9)	-4(8)	13(7)
C(8A)	181(10)	215(12)	243(13)	-14(10)	13(9)	22(9)
C(9A)	219(11)	383(15)	285(14)	-82(12)	-78(10)	68(11)
C(10A)	144(10)	232(13)	464(17)	8(12)	13(11)	-14(9)
C(11A)	226(10)	246(12)	195(12)	-19(10)	11(9)	78(9)
C(12A)	300(12)	328(15)	165(13)	-10(11)	-51(10)	109(10)
Br(2)	218(1)	328(1)	391(1)	-72(1)	103(1)	-69(1)
S(1B)	214(2)	155(2)	113(2)	11(2)	14(2)	-32(2)
O(1B)	891(14)	204(9)	562(13)	138(9)	-162(11)	11(9)
O(2B)	255(7)	246(8)	155(7)	16(6)	-34(6)	4(6)
N(1B)	188(8)	154(9)	136(9)	18(7)	44(7)	-40(7)
C(1B)	262(10)	205(11)	113(10)	-56(9)	32(8)	-59(8)
C(2B)	429(13)	203(12)	161(11)	-10(9)	22(10)	-151(10)
C(3B)	606(16)	168(12)	238(13)	-30(10)	-127(11)	8(11)
C(4B)	332(12)	240(13)	381(15)	-76(11)	-51(11)	61(10)
C(5B)	238(11)	227(12)	258(13)	-50(10)	27(9)	-3(9)
C(6B)	209(8)	128(9)	139(10)	-23(9)	16(7)	-39(8)
C(7B)	266(10)	142(10)	160(11)	-20(9)	49(8)	-43(8)
C(8B)	329(12)	156(11)	308(15)	-10(11)	112(11)	-67(10)
C(9B)	643(18)	193(13)	217(14)	-72(11)	106(13)	5(13)
C(10B)	287(11)	241(13)	348(15)	23(11)	100(11)	23(10)
C(11B)	264(10)	222(11)	159(11)	5(10)	52(9)	-70(9)
C(12B)	394(13)	294(14)	168(13)	-100(11)	40(11)	-97(11)
Br(3)	447(1)	242(1)	407(1)	120(1)	172(1)	27(1)
S(1C)	177(2)	196(3)	126(3)	-15(2)	14(2)	-28(2)
O(1C)	475(10)	492(11)	495(12)	-84(9)	-280(9)	137(9)
O(2C)	249(7)	195(7)	225(8)	60(6)	19(6)	-42(6)
N(1C)	177(8)	202(9)	133(9)	-32(7)	15(7)	6(7)
C(1C)	212(9)	196(10)	196(11)	40(9)	75(8)	45(9)
C(2C)	194(9)	192(11)	356(13)	-75(11)	35(9)	-26(10)
C(3C)	223(10)	322(13)	257(13)	-59(11)	-59(9)	109(9)
C(4C)	287(11)	239(12)	225(12)	82(10)	41(10)	116(9)
C(5C)	251(11)	163(11)	278(13)	-4(10)	72(9)	8(9)

C(6C)	161(9)	208(10)	135(10)	1(9)	21(8)	23(8)
C(7C)	235(10)	162(10)	189(11)	-26(8)	55(8)	1(8)
C(8C)	257(10)	263(13)	248(13)	-48(11)	6(9)	77(10)
C(9C)	260(12)	326(14)	254(13)	-74(11)	88(10)	-11(10)
C(10C)	400(13)	183(12)	442(16)	-32(13)	156(12)	16(11)
C(11C)	278(11)	307(13)	199(12)	-55(11)	26(9)	22(10)
C(12C)	343(13)	357(15)	277(14)	-61(12)	79(11)	108(11)

Table A2.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for RUN02 (CCDC 780836).

	x	y	z	U_{iso}
H(1A)	680(17)	9690(10)	10696(14)	1(5)
H(2A)	2878(17)	7459(10)	9401(14)	23(6)
H(4A)	4585(19)	9508(11)	9152(14)	32(6)
H(5A)	3230(16)	10006(9)	10348(13)	13(5)
H(8A1)	-1307(19)	10787(11)	9363(15)	32(6)
H(8A2)	-1397(18)	10393(10)	10416(15)	24(5)
H(8A3)	-2715(18)	10554(10)	9553(14)	25(5)
H(9A1)	-3050(20)	9806(11)	7845(16)	43(7)
H(9A2)	-1970(20)	9295(12)	7475(16)	49(7)
H(9A3)	-1707(19)	10087(10)	7534(15)	27(6)
H(10A)	-1772(18)	8989(10)	10362(15)	23(6)
H(10B)	-1812(19)	8532(11)	9239(16)	35(6)
H(10C)	-2966(19)	8987(10)	9466(14)	22(5)
H(11A)	1808(16)	8876(9)	12208(13)	9(5)
H(11B)	2591(18)	9603(11)	12058(14)	27(6)
H(12A)	3719(16)	8132(9)	12208(13)	16(5)
H(12B)	3999(17)	8716(10)	12986(15)	19(6)
H(12C)	4600(20)	8842(11)	12008(16)	37(7)
H(1B)	2260(17)	441(10)	7606(13)	14(5)
H(2B)	4155(17)	2724(10)	6114(13)	18(5)
H(4B)	224(17)	2638(11)	6600(14)	28(5)
H(5B)	844(18)	1619(11)	7647(14)	26(6)
H(8B1)	1589(18)	-1388(11)	6532(15)	22(5)
H(8B2)	751(18)	-732(10)	6410(15)	21(6)
H(8B3)	1897(19)	-781(11)	7420(16)	35(6)
H(9B1)	2860(20)	-511(11)	4366(15)	35(6)
H(9B2)	1340(20)	-670(13)	4447(19)	63(9)
H(9B3)	2350(18)	-1206(11)	4625(15)	24(6)
H(10D)	4325(19)	-557(11)	7037(16)	31(6)
H(10E)	4640(20)	-503(12)	5916(17)	46(7)
H(10F)	4188(18)	-1241(12)	6290(16)	33(6)
H(11C)	2666(18)	1320(11)	9099(14)	28(6)
H(11D)	4213(17)	1188(10)	8913(14)	28(5)
H(12D)	4276(19)	2590(12)	8910(14)	44(6)
H(12E)	3795(16)	2316(10)	9895(14)	17(5)
H(12F)	2760(20)	2679(13)	9065(15)	47(7)
H(1C)	-61(17)	5901(10)	5955(14)	19(5)
H(2C)	4390(19)	6797(10)	7546(16)	33(7)
H(4C)	3426(18)	4836(10)	8550(14)	19(6)
H(5C)	1695(18)	4768(10)	7196(14)	24(6)
H(8C1)	-3048(18)	6886(10)	6336(14)	26(6)
H(8C2)	-2699(17)	6101(10)	6516(14)	17(5)
H(8C3)	-1971(17)	6612(10)	5679(14)	23(5)
H(9C1)	-1266(16)	7081(10)	8972(13)	18(5)
H(9C2)	-2431(18)	6514(11)	8445(14)	30(6)
H(9C3)	-2649(19)	7294(11)	8168(15)	35(6)

H(10G)	-172(18)	7526(11)	6447(15)	29(6)
H(10H)	43(19)	7728(12)	7665(15)	41(7)
H(10I)	-1299(18)	7979(10)	6953(14)	21(5)
H(11E)	1320(20)	4978(11)	5276(16)	41(7)
H(11F)	1625(17)	5765(10)	4720(14)	16(5)
H(12G)	4043(18)	5574(10)	5207(14)	25(6)
H(12H)	3370(20)	4825(13)	4412(19)	71(8)
H(12I)	3640(20)	4733(12)	5633(19)	55(8)

Table A2.6. Hydrogen bonds for RUN02 (CCDC 780836) [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1A)-H(1A)...O(2C)#1	0.692(16)	2.219(16)	2.897(2)	167(2)
N(1B)-H(1B)...O(2A)#2	0.802(17)	2.148(17)	2.9066(19)	158.0(17)
N(1C)-H(1C)...O(2B)#3	0.876(17)	2.001(17)	2.834(2)	158.6(16)

Symmetry transformations used to generate equivalent atoms:
#1 -x,y+1/2,-z+2
#2 x,y-1,z
#3 -x,y+1/2,-z+1