Supplementary Material for Organic & Biomolecular Chemistry

Supplementary data

4-(Tetrahydro-*4H*-thiopyran-1-oxide-4-ylidene)-cyclohexanone oxime in the solid state. A two-dimensional network of enantiomorphous chains interconnected by weak hydrogen bonds

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† Electronic Supplementary Information

PM3 Archive files for an enantiomer of **1**, *viz.* **1**-*R*, with its bicyclohexylidene skeleton in either a *syn* or *anti*-conformation. Single-crystal X-ray structure data of $\mathbf{(1)_4 \cdot C_6H_6}$ and observed and calculated structure factors (CCDC Number: 260603). See http://www.rsc.org/suppdata/xxxxx

SUMMARY OF PM3 CALCULATION

syn 4-(tetrahydro-4H-thiopyran-1-oxide-4-ylidene)cyclohexanon oxim (*syn*-**1**-*R*)

C11H17NO2S

GEOMETRY OPTIMISED USING EIGENVECTOR FOLLOWING (EF).
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-33.724877 KCAL
ELECTRONIC ENERGY	=	-15821.182554 EV
CORE-CORE REPULSION	=	13321.325830 EV
DIPOLE	=	3.74489 DEBYE
NO. OF FILLED LEVELS	=	42
IONIZATION POTENTIAL	=	9.263129 EV
MOLECULAR WEIGHT	=	227.321
SCF CALCULATIONS	=	93

COMPUTATION TIME = 1 MINUTES AND 9.590 SECONDS

FINAL GEOMETRY OBTAINED CHARGE

PM3 EF HESS=1 PRECISE NOINTER T=8H

syn 4-(tetrahydro-4H-thiopyran-1-oxide-4-ylidene)cyclohexanon oxim (*syn*-**1**-*R*)

C	.0000000	0	.000000	0	.000000	0	0	0	0	-.1060
C	1.3447521	1	.000000	0	.000000	0	1	0	0	-.1364
C	1.4991276	1	123.262785	1	.000000	0	2	1	0	-.0521
C	1.5163516	1	111.552914	1	115.985106	1	3	2	1	-.3266
S	1.8402069	1	115.660295	1	56.810120	1	4	3	2	.9021
C	1.8401887	1	98.930090	1	-43.528543	1	5	4	3	-.3266
C	1.5163366	1	115.657989	1	43.529940	1	6	5	4	-.0522
C	1.4970129	1	123.644334	1	-.314164	1	1	2	3	-.0610
C	1.4970862	1	123.664948	1	178.793618	1	1	2	3	-.0637
C	1.5233726	1	111.033330	1	124.039939	1	9	1	2	-.0563
C	1.5038156	1	110.796357	1	52.158011	1	10	9	1	-.0772
C	1.4998194	1	115.550323	1	-50.660035	1	11	10	9	-.0672
N	1.2999335	1	117.591410	1	130.142832	1	11	10	9	-.0297
O	1.3994651	1	118.579955	1	179.058744	1	13	11	10	-.2613
H	1.1079154	1	112.566579	1	173.013356	1	12	11	10	.0738
H	1.1090810	1	107.912902	1	-70.578874	1	12	11	10	.0634
H	1.1117615	1	111.597358	1	-1.826811	1	8	1	2	.0640
H	1.1088882	1	108.415657	1	114.139418	1	8	1	2	.0647
H	1.1101900	1	108.900180	1	-121.914983	1	3	2	1	.0817
H	1.1126524	1	111.145423	1	-6.075602	1	3	2	1	.0655
H	1.1056403	1	110.129458	1	-64.496525	1	4	3	2	.0867
H	1.1057348	1	109.446818	1	178.977446	1	4	3	2	.0983
O	1.5584825	1	105.454362	1	65.338409	1	5	4	3	-.6911
H	1.1056496	1	106.904187	1	-79.493251	1	6	5	4	.0868
H	1.1057347	1	107.960347	1	166.486133	1	6	5	4	.0983
H	1.1101870	1	110.403255	1	64.416409	1	7	6	5	.0817
H	1.1126652	1	109.146857	1	179.985117	1	7	6	5	.0658
H	1.1117123	1	111.616834	1	1.591826	1	9	1	2	.0638
H	1.1088194	1	108.493315	1	-114.431555	1	9	1	2	.0648
H	1.1083990	1	109.630825	1	176.536975	1	10	9	1	.0716
H	1.1090853	1	110.185515	1	-67.281202	1	10	9	1	.0598
H	.9509176	1	100.620780	1	179.211764	1	14	13	11	.2148

SUMMARY OF PM3 CALCULATION

anti 4-(tetrahydro-4H-thiopyran-1-oxide-4-ylidene)cyclohexanon oxime (*anti*-**1**-*R*)

C11H17NO2S

GEOMETRY OPTIMISED USING EIGENVECTOR FOLLOWING (EF).
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-33.298489 KCAL
ELECTRONIC ENERGY	=	-15687.127966 EV
CORE-CORE REPULSION	=	13187.289731 EV
DIPOLE	=	4.32362 DEBYE
NO. OF FILLED LEVELS	=	42
IONIZATION POTENTIAL	=	9.311107 EV
MOLECULAR WEIGHT	=	227.321
SCF CALCULATIONS	=	48

COMPUTATION TIME = 17 MINUTES AND 41.710 SECONDS

FINAL GEOMETRY OBTAINED CHARGE
PM3 EF HESS=1 PRECISE NOINTER T=8H
anti 4-(tetrahydro-4H-thiopyran-1-oxide-4-ylidene)cyclohexanon oxime (anti-**1**-*R*)

C	.0000000	0	.000000	0	.000000	0	0	0	0	-.0623
C	1.4971176	1	.000000	0	.000000	0	1	0	0	-.0921
C	1.3449280	1	123.501251	1	.000000	0	2	1	0	-.1473
C	1.4989849	1	123.333631	1	-179.636212	1	3	2	1	-.0394
C	1.4989662	1	123.353243	1	.733703	1	3	2	1	-.0394
C	1.5164310	1	111.532652	1	114.147896	1	4	3	2	-.3354
C	1.5164065	1	111.525544	1	-114.126335	1	5	3	2	-.3355
S	1.8431265	1	113.023026	1	59.329054	1	6	4	3	.9045
C	1.5236808	1	111.598469	1	-125.693121	1	1	2	3	-.0680
C	1.4971742	1	123.524179	1	178.954520	1	2	3	1	-.0650
C	1.4993467	1	110.896195	1	-51.308276	1	9	1	2	-.0779
C	1.5033008	1	115.372869	1	50.846039	1	11	9	1	-.0572
N	1.2998245	1	126.937067	1	-130.034720	1	11	9	1	-.0282
O	1.3992327	1	118.579738	1	-.012191	1	13	11	9	-.2610
H	1.1118655	1	111.578570	1	-3.234020	1	1	2	3	.0638
H	1.1088767	1	108.249512	1	112.655905	1	1	2	3	.0664
H	1.1096449	1	108.943625	1	-123.384279	1	4	3	2	.0620
H	1.1127508	1	111.101862	1	-7.713041	1	4	3	2	.0677
H	1.1096721	1	108.941959	1	123.411166	1	5	3	2	.0620
H	1.1127511	1	111.116652	1	7.742653	1	5	3	2	.0674
H	1.1065617	1	110.331221	1	-65.234023	1	6	4	3	.0990
H	1.1061234	1	109.997704	1	178.815805	1	6	4	3	.0949
O	1.5606577	1	103.661007	1	-154.705238	1	8	6	4	-.6909
H	1.1065691	1	110.330376	1	65.188682	1	7	5	3	.0990
H	1.1061083	1	109.997807	1	-178.859209	1	7	5	3	.0948
H	1.1079477	1	109.195571	1	-175.935304	1	9	1	2	.0742
H	1.1090910	1	110.303309	1	68.179503	1	9	1	2	.0653
H	1.1118082	1	111.598561	1	3.006270	1	10	2	3	.0636
H	1.1088123	1	108.320896	1	-112.938117	1	10	2	3	.0666
H	1.1084374	1	112.222005	1	-174.042939	1	12	11	9	.0720
H	1.1090745	1	107.983641	1	69.607899	1	12	11	9	.0617
H	.9509387	1	100.633815	1	179.288057	1	14	13	11	.2150

Table S1 - Crystal Data and Details of the Structure Determination

Crystal Data			
Empirical Formula	4(C11 H17 N O2 S), C6 H6		
Formula Weight	987.41		
Crystal System	Triclinic		
Space group	P-1	(No. 2)	
a, b, c [Angstrom]	5.0885(3)	15.5224(17)	16.5379(16)
alpha, beta, gamma [deg]	102.839(8)	95.947(6)	94.025(7)
V [Ang**3]	1260.9(2)		
Z	1		
D(calc) [g/cm**3]	1.300		
F(000)	530		
Mu(MoKa) [/mm]	0.2		
Crystal Size [mm]	0.05 x	0.50 x	0.62
Data Collection			
Temperature (K)	150		
Radiation [Angstrom]	MoKa	0.71073	
Theta Min-Max [Deg]	1.3,	27.5	
Scan,(Type & Range) [Deg]	0.77 + 0.35 Tan(Theta)		
Dataset	-6: 4 ; -20: 20 ; -21: 21		
Tot., Uniq. Data, R(int)	7139,	5799,	0.116
Observed data [I > 2.0 sigma(I)]	3386		
Refinement			
Nref, Npar	5799,	300	
R, wR, S	0.1010, 0.2801, 1.03		
w = 1/[^2^(FO^2^)+(0.1000P)^2^+4.6080P] WHERE P=(FO^2^+2FC^2^)/3'			
Max. and Av. Shift/Error	0.61, 0.01		
Min. and Max. resd. dens. [e/Ang^3]	-0.75, 1.33		

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms

Atom	x	y	z	U(eq) [Ang^2]
S1'	0.8130(3)	0.25987(9)	0.19739(9)	0.0322(4)
O1	0.2625(9)	0.7514(3)	0.5077(3)	0.0529(17)
O1'	1.1120(7)	0.2643(3)	0.1982(2)	0.0353(11)
N1	0.2975(12)	0.7452(4)	0.4250(4)	0.060(2)
C1	0.4103(19)	0.6704(6)	0.4000(5)	0.076(3)
C2	0.493(2)	0.6020(6)	0.4462(5)	0.084(4)
C2'	0.7619(10)	0.3037(4)	0.3041(3)	0.0314(17)
C3	0.7456(17)	0.5727(5)	0.4284(4)	0.062(3)
C3'	0.9157(11)	0.3941(4)	0.3412(3)	0.0340(17)
C4	0.7622(16)	0.5434(4)	0.3351(4)	0.052(2)
C4'	0.8360(11)	0.4650(4)	0.2972(3)	0.0337(17)
C5	0.6939(19)	0.6178(5)	0.2928(5)	0.072(3)
C5'	0.8707(11)	0.4398(3)	0.2047(3)	0.0303(17)
C6	0.444(2)	0.6487(6)	0.3082(6)	0.088(4)
C6'	0.7101(11)	0.3529(4)	0.1585(3)	0.0332(17)
S11'	0.7733(3)	-0.08750(10)	0.56513(9)	0.0361(4)
O11	0.2345(9)	0.1582(3)	1.0547(3)	0.0559(17)
O11'	1.0705(7)	-0.0919(3)	0.5680(2)	0.0375(11)
N11	0.2904(10)	0.2086(4)	0.9991(4)	0.051(2)
C11	0.3622(10)	0.1532(4)	0.9310(4)	0.0414(19)
C12	0.3917(11)	0.0576(4)	0.9159(4)	0.0398(19)
C12'	0.6898(11)	-0.1193(4)	0.6582(4)	0.0380(19)
C13	0.6772(11)	0.0402(4)	0.8957(4)	0.0384(19)
C13'	0.8584(11)	-0.0653(4)	0.7365(4)	0.0330(17)
C14	0.7404(10)	0.0787(4)	0.8234(3)	0.0304(16)
C14'	0.8204(10)	0.0326(3)	0.7529(3)	0.0276(16)
C15	0.7111(10)	0.1775(4)	0.8423(4)	0.0362(17)
C15'	0.8903(10)	0.0720(4)	0.6818(3)	0.0307(17)
C16	0.4329(11)	0.1976(4)	0.8643(4)	0.0406(17)
C16'	0.7252(10)	0.0277(4)	0.5990(3)	0.0334(17)
C20	0.102(3)	0.5758(7)	0.0523(7)	0.093(4)
C21	0.118(3)	0.4255(8)	-0.0006(8)	0.092(5)
C22	0.2182(16)	0.5008(12)	0.0513(7)	0.090(5)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters

Atom	x	y	z	U(iso) [Ang^2]
H1	0.14910	0.81800	0.53510	0.1000
H2A	0.50030	0.62680	0.50580	0.1010
H2B	0.35980	0.55140	0.43130	0.1010
H3A	0.77880	0.52360	0.45420	0.0750
H3B	0.88300	0.62070	0.45280	0.0750
H5A	0.83060	0.66710	0.31230	0.0860
H5B	0.69430	0.59700	0.23300	0.0860
H6A	0.30400	0.60370	0.27840	0.1060
H6B	0.42420	0.70140	0.28660	0.1060
H21'	0.57410	0.30910	0.30680	0.0380
H22'	0.81640	0.26240	0.33730	0.0380
H31'	0.88880	0.41260	0.39950	0.0410
H32'	1.10360	0.38840	0.33900	0.0410
H51'	1.05710	0.43440	0.19920	0.0370
H52'	0.81660	0.48700	0.17880	0.0370
H61'	0.72990	0.34260	0.09950	0.0400
H62'	0.52370	0.35800	0.16430	0.0400
H11	0.12530	0.20640	1.09670	0.8(4)
H12A	0.26380	0.02570	0.86940	0.0480
H12B	0.35740	0.03620	0.96500	0.0480
H12C	0.50430	-0.11160	0.66350	0.0460
H12D	0.71320	-0.18170	0.65310	0.0460
H13A	0.81390	-0.08790	0.78400	0.0400
H13B	1.04390	-0.07290	0.73110	0.0400
H13C	0.80360	0.06690	0.94440	0.0460
H13D	0.69220	-0.02320	0.88210	0.0460
H15A	1.07660	0.06660	0.67590	0.0370
H15B	0.86510	0.13470	0.69510	0.0370
H15C	0.74530	0.20040	0.79400	0.0430
H15D	0.84200	0.20750	0.88870	0.0430
H16A	0.77200	0.05850	0.55670	0.0400
H16B	0.53900	0.03330	0.60470	0.0400
H16C	0.42830	0.26120	0.88320	0.0480
H16D	0.30430	0.17690	0.81490	0.0480

H20	0.17390	0.62860	0.08900	0.1120
H21	0.19970	0.37370	-0.00090	0.1100
H22	0.37140	0.50180	0.08760	0.1080

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table S4 - (An)isotropic Displacement Parameters

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
S1'	0.0291(7)	0.0277(7)	0.0369(7)	0.0016(5)	0.0064(5)	-0.0006(5)
O1	0.053(3)	0.053(3)	0.051(3)	0.013(2)	0.006(2)	-0.009(2)
O1'	0.0263(18)	0.040(2)	0.039(2)	0.0023(18)	0.0108(16)	0.0112(16)
N1	0.066(4)	0.071(4)	0.039(3)	0.007(3)	0.009(3)	-0.013(3)
C1	0.103(7)	0.064(5)	0.072(6)	0.017(4)	0.035(5)	0.050(5)
C2	0.132(8)	0.084(6)	0.052(5)	0.018(4)	0.048(5)	0.054(6)
C2'	0.029(3)	0.036(3)	0.034(3)	0.013(2)	0.013(2)	0.006(2)
C3	0.097(6)	0.058(4)	0.036(4)	0.009(3)	0.021(4)	0.023(4)
C3'	0.039(3)	0.034(3)	0.031(3)	0.007(2)	0.011(2)	0.009(2)
C4	0.091(5)	0.039(3)	0.035(3)	0.014(3)	0.023(3)	0.022(3)
C4'	0.045(3)	0.031(3)	0.027(3)	0.009(2)	0.007(2)	0.006(2)
C5	0.125(8)	0.047(4)	0.056(5)	0.019(4)	0.033(5)	0.035(5)
C5'	0.033(3)	0.029(3)	0.030(3)	0.005(2)	0.012(2)	0.004(2)
C6	0.130(9)	0.080(6)	0.076(6)	0.033(5)	0.038(6)	0.069(6)
C6'	0.031(3)	0.036(3)	0.032(3)	0.006(2)	0.006(2)	0.002(2)
S11'	0.0268(7)	0.0416(8)	0.0345(7)	-0.0028(6)	0.0070(5)	-0.0013(6)
O11	0.045(3)	0.053(3)	0.072(3)	0.017(3)	0.010(2)	0.009(2)
O11'	0.0274(19)	0.041(2)	0.040(2)	-0.0022(18)	0.0108(16)	0.0031(16)
N11	0.032(3)	0.059(4)	0.067(4)	0.031(3)	-0.004(3)	-0.006(2)
C11	0.023(3)	0.064(4)	0.031(3)	-0.005(3)	0.003(2)	0.013(3)
C12	0.030(3)	0.057(4)	0.035(3)	0.015(3)	0.009(2)	0.000(3)
C12'	0.029(3)	0.034(3)	0.052(4)	0.007(3)	0.017(3)	0.001(2)
C13	0.033(3)	0.053(4)	0.034(3)	0.014(3)	0.013(2)	0.012(3)
C13'	0.033(3)	0.032(3)	0.037(3)	0.011(2)	0.010(2)	0.006(2)
C14	0.022(2)	0.038(3)	0.032(3)	0.008(2)	0.005(2)	0.006(2)
C14'	0.023(2)	0.033(3)	0.029(3)	0.010(2)	0.006(2)	0.004(2)
C15	0.027(3)	0.039(3)	0.039(3)	0.000(2)	0.007(2)	0.003(2)

C15'	0.032(3)	0.030(3)	0.030(3)	0.004(2)	0.010(2)	0.003(2)
C16	0.031(3)	0.040(3)	0.047(3)	-0.001(3)	0.008(2)	0.009(2)
C16'	0.027(3)	0.044(3)	0.032(3)	0.011(2)	0.010(2)	0.006(2)
C20	0.145(10)	0.050(5)	0.077(7)	-0.006(5)	0.059(7)	-0.047(6)
C21	0.136(10)	0.086(7)	0.101(8)	0.068(7)	0.089(8)	0.076(7)
C22	0.039(4)	0.171(12)	0.071(6)	0.049(8)	0.015(4)	0.003(6)

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and h(i) are the Reflection Indices.

Table S5 - Bond Distances (Angstrom)

S1'	-O1'	1.517(4)	C3	-H3A	0.9691
S1'	-C2'	1.798(5)	C3'	-H32'	0.9700
S1'	-C6'	1.795(6)	C3'	-H31'	0.9699
S11'	-C12'	1.799(7)	C5	-H5A	0.9709
S11'	-C16'	1.793(6)	C5	-H5B	0.9700
S11'	-O11'	1.515(4)	C5'	-H51'	0.9698
O1	-N1	1.381(8)	C5'	-H52'	0.9692
O1	-H1	1.2397	C6	-H6B	0.9700
O11	-N11	1.372(8)	C6	-H6A	0.9709
O11	-H11	1.1218	C6'	-H62'	0.9701
N1	-C1	1.333(11)	C6'	-H61'	0.9701
N11	-C11	1.357(9)	C11	-C12	1.470(9)
C1	-C2	1.498(13)	C11	-C16	1.485(9)
C1	-C6	1.511(13)	C12	-C13	1.553(8)
C2	-C3	1.431(13)	C12'	-C13'	1.517(9)
C2'	-C3'	1.524(8)	C13	-C14	1.503(8)
C3	-C4	1.522(9)	C13'	-C14'	1.513(8)
C3'	-C4'	1.504(8)	C14	-C14'	1.344(7)
C4	-C5	1.520(10)	C14	-C15	1.517(9)
C4	-C4'	1.337(9)	C14'	-C15'	1.503(7)
C4'	-C5'	1.524(7)	C15	-C16	1.534(8)
C5	-C6	1.418(14)	C15'	-C16'	1.522(7)
C5'	-C6'	1.526(8)	C12	-H12A	0.9705

C2	-H2A	0.9710	C12	-H12B	0.9702
C2	-H2B	0.9704	C12'	-H12C	0.9702
C2'	-H22'	0.9691	C12'	-H12D	0.9703
C2'	-H21'	0.9699	C13	-H13C	0.9701
C3	-H3B	0.9704	C13	-H13D	0.9699
C13'	-H13A	0.9693	C16'	-H16A	0.9705
C13'	-H13B	0.9702	C16'	-H16B	0.9698
C15	-H15C	0.9701	C20	-C22	1.34(2)
C15	-H15D	0.9701	C20	-C21_a	1.33(2)
C15'	-H15A	0.9705	C21	-C22	1.32(2)
C15'	-H15B	0.9697	C20	-H20	0.9299
C16	-H16C	0.9698	C21	-H21	0.9300
C16	-H16D	0.9705	C22	-H22	0.9303

Table S6 - Bond Angles (Degrees)

O1'	-S1'	-C2'	105.0(2)	C3	-C2	-H2A	109.18
O1'	-S1'	-C6'	106.0(3)	C3	-C2	-H2B	109.19
C2'	-S1'	-C6'	96.3(3)	C1	-C2	-H2A	108.96
C12'	-S11'	-C16'	96.4(3)	H2A	-C2	-H2B	107.72
O11'	-S11'	-C16'	106.1(3)	S1'	-C2'	-H22'	109.04
O11'	-S11'	-C12'	104.8(2)	C3'	-C2'	-H21'	109.02
N1	-O1	-H1	110.70	S1'	-C2'	-H21'	109.01
N11	-O11	-H11	98.87	C3'	-C2'	-H22'	109.12
O1	-N1	-C1	106.6(6)	H21'	-C2'	-H22'	107.95
O11	-N11	-C11	107.3(5)	C4	-C3	-H3B	108.97
C2	-C1	-C6	115.0(8)	H3A	-C3	-H3B	107.92
N1	-C1	-C2	130.9(7)	C2	-C3	-H3A	109.11
N1	-C1	-C6	114.0(8)	C2	-C3	-H3B	109.06
C1	-C2	-C3	112.7(8)	C4	-C3	-H3A	109.10
S1'	-C2'	-C3'	112.6(4)	C2'	-C3'	-H32'	108.87
C2	-C3	-C4	112.6(7)	C4'	-C3'	-H31'	108.81
C2'	-C3'	-C4'	113.7(4)	C4'	-C3'	-H32'	108.79
C3	-C4	-C4'	124.6(6)	C2'	-C3'	-H31'	108.78
C3	-C4	-C5	109.8(6)	H31'	-C3'	-H32'	107.71
C4'	-C4	-C5	125.5(6)	H5A	-C5	-H5B	107.71

C3'	-C4'	-C5'	111.7(5)	C6	-C5	-H5A	108.82
C3'	-C4'	-C4	124.5(5)	C4	-C5	-H5A	108.86
C4	-C4'	-C5'	123.6(5)	C4	-C5	-H5B	108.94
C4	-C5	-C6	113.5(8)	C6	-C5	-H5B	108.87
C4'	-C5'	-C6'	112.9(4)	H51'	-C5'	-H52'	107.82
C1	-C6	-C5	112.7(8)	C4'	-C5'	-H52'	108.93
S1'	-C6'	-C5'	112.3(4)	C6'	-C5'	-H51'	108.99
C1	-C2	-H2B	108.97	C4'	-C5'	-H51'	109.03
C6'	-C5'	-H52'	109.02	C11	-C12	-H12A	109.69
C1	-C6	-H6B	109.00	C11	-C12	-H12B	109.73
C5	-C6	-H6A	109.21	C13	-C12	-H12A	109.64
C5	-C6	-H6B	109.24	C13	-C12	-H12B	109.74
H6A	-C6	-H6B	107.61	H12A	-C12	-H12B	108.21
C1	-C6	-H6A	108.98	S11'	-C12'	-H12C	109.09
C5'	-C6'	-H61'	109.12	S11'	-C12'	-H12D	109.14
C5'	-C6'	-H62'	109.12	C13'	-C12'	-H12C	109.02
S1'	-C6'	-H61'	109.17	C13'	-C12'	-H12D	109.10
S1'	-C6'	-H62'	109.14	H12C	-C12'	-H12D	107.88
H61'	-C6'	-H62'	107.91	C12	-C13	-H13C	109.53
N11	-C11	-C12	129.4(6)	C12	-C13	-H13D	109.54
N11	-C11	-C16	114.3(6)	C14	-C13	-H13C	109.58
C12	-C11	-C16	116.1(5)	C14	-C13	-H13D	109.65
C11	-C12	-C13	109.8(5)	H13C	-C13	-H13D	108.10
S11'	-C12'	-C13'	112.5(4)	C12'	-C13'	-H13A	108.99
C12	-C13	-C14	110.4(5)	C12'	-C13'	-H13B	108.98
C12'	-C13'	-C14'	112.9(5)	C14'	-C13'	-H13A	109.06
C13	-C14	-C15	110.6(5)	C14'	-C13'	-H13B	109.06
C14'	-C14	-C15	124.6(5)	H13A	-C13'	-H13B	107.73
C13	-C14	-C14'	124.7(5)	C14	-C15	-H15C	109.21
C13'	-C14'	-C15'	111.6(4)	C14	-C15	-H15D	109.22
C14	-C14'	-C15'	124.5(5)	C16	-C15	-H15C	109.30
C13'	-C14'	-C14	123.9(5)	C16	-C15	-H15D	109.24
C14	-C15	-C16	111.8(5)	H15C	-C15	-H15D	107.98
C14'	-C15'	-C16'	113.1(5)	C14'	-C15'	-H15A	108.90
C11	-C16	-C15	110.3(5)	C14'	-C15'	-H15B	108.93
S11'	-C16'	-C15'	112.7(4)	C16'	-C15'	-H15A	108.92

C16'	-C15'	-H15B	109.02	H16A	-C16'	-H16B	107.77
H15A	-C15'	-H15B	107.81	C21_a	-C20	-C22	119.7(11)
C11	-C16	-H16C	109.60	C20_a	-C21	-C22	119.5(13)
C11	-C16	-H16D	109.71	C20	-C22	-C21	120.8(11)
C15	-C16	-H16C	109.59	C22	-C20	-H20	120.29
C15	-C16	-H16D	109.58	C21_a	-C20	-H20	119.96
H16C	-C16	-H16D	108.05	C22	-C21	-H21	120.30
S11'	-C16'	-H16A	109.12	C20_a	-C21	-H21	120.24
S11'	-C16'	-H16B	109.12	C20	-C22	-H22	119.61
C15'	-C16'	-H16A	108.98	C21	-C22	-H22	119.59
C15'	-C16'	-H16B	109.03				

Table S7 - Torsion Angles (Degrees)

O1'	-S1'	-C2'	-C3'	52.3(5)
C6'	-S1'	-C2'	-C3'	-56.1(4)
O1'	-S1'	-C6'	-C5'	-50.7(4)
C2'	-S1'	-C6'	-C5'	56.8(4)
C12'	-S11'	-C16'	-C15'	55.6(4)
O11'	-S11'	-C12'	-C13'	52.7(5)
C16'	-S11'	-C12'	-C13'	-55.9(5)
O11'	-S11'	-C16'	-C15'	-51.9(4)
O1	-N1	-C1	-C2	-0.3(12)
O1	-N1	-C1	-C6	175.4(7)
O11	-N11	-C11	-C16	-179.4(5)
O11	-N11	-C11	-C12	-2.6(8)
C6	-C1	-C2	-C3	46.7(11)
C2	-C1	-C6	-C5	-45.9(11)
N1	-C1	-C2	-C3	-137.7(10)
N1	-C1	-C6	-C5	137.7(8)
C1	-C2	-C3	-C4	-51.7(9)
S1'	-C2'	-C3'	-C4'	61.9(5)
C2	-C3	-C4	-C5	55.3(9)
C2	-C3	-C4	-C4'	-127.1(9)
C2'	-C3'	-C4'	-C5'	-58.0(6)
C2'	-C3'	-C4'	-C4	126.6(7)

C3	-C4	-C5	-C6	-55.0(9)
C4'	-C4	-C5	-C6	127.4(9)
C3	-C4	-C4'	-C5'	-175.3(6)
C5	-C4	-C4'	-C5'	1.9(11)
C3	-C4	-C4'	-C3'	-0.5(11)
C5	-C4	-C4'	-C3'	176.8(7)
C3'	-C4'	-C5'	-C6'	58.5(6)
C4	-C4'	-C5'	-C6'	-126.1(7)
C4	-C5	-C6	-C1	50.4(10)
C4'	-C5'	-C6'	-S1'	-62.9(5)
C16	-C11	-C12	-C13	53.8(7)
N11	-C11	-C12	-C13	-122.9(6)
N11	-C11	-C16	-C15	125.1(6)
C12	-C11	-C16	-C15	-52.1(7)
C11	-C12	-C13	-C14	-55.3(7)
S11'	-C12'	-C13'	-C14'	62.6(6)
C12	-C13	-C14	-C15	57.7(6)
C12	-C13	-C14	-C14'	-124.4(6)
C12'	-C13'	-C14'	-C14	122.0(6)
C12'	-C13'	-C14'	-C15'	-59.5(6)
C13	-C14	-C14'	-C13'	-0.1(8)
C13	-C14	-C14'	-C15'	-178.3(5)
C13	-C14	-C15	-C16	-56.5(6)
C14'	-C14	-C15	-C16	125.6(6)
C15	-C14	-C14'	-C13'	177.6(5)
C15	-C14	-C14'	-C15'	-0.6(8)
C13'	-C14'	-C15'	-C16'	59.2(6)
C14	-C14'	-C15'	-C16'	-122.4(6)
C14	-C15	-C16	-C11	51.7(7)
C14'	-C15'	-C16'	-S11'	-62.3(5)
C21_a	-C20	-C22	-C21	0.3(19)
C22	-C20	-C21_a	-C22_a	0(2)
C20_a	-C21	-C22	-C20	0(2)

Table S8 - Contact Distances(Angstrom)

S11'	.O1_k	3.381(5)	O11'	.H16A_h	2.4338
S1'	.H11_b	2.4711	O11'	.H1_l	1.4824
S11'	.H1_l	2.5143	N1	.H3B_e	2.9014
O1	.O11'_d	2.706(6)	N1	.H5A_e	2.8744
O1	.C12'_c	3.316(8)	N11	.H21_q	2.6357
O1	.S11'_c	3.381(5)	N11	.H15D_n	2.7672
O1	.C2'_f	3.418(7)	C2'	.O1_f	3.418(7)
O1'	.O11_b	2.729(6)	C5'	.C22_i	3.496(13)
O11	.O1'_m	2.729(6)	C11	.C14_n	3.453(8)
O11	.C13_o	3.406(8)	C11	.C15_n	3.562(8)
O11'	.C16'_h	3.373(6)	C12	.C14_n	3.571(8)
O11'	.O1_l	2.706(6)	C12'	.O1_k	3.316(8)
O1	.H3B_e	2.6339	C13	.O11_o	3.406(8)
O1	.H2A	2.3485	C14	.C12_p	3.571(8)
O1	.H22'_f	2.6876	C14	.C11_p	3.453(8)
O1'	.H32'	2.6783	C15	.C11_p	3.562(8)
O1'	.H21'_g	2.7529	C16'	.O11'_h	3.373(6)
O1'	.H11_b	1.7296	C22	.C22_t	3.479(13)
O1'	.H51'	2.6711	C22	.C5'_e	3.496(13)
O1'	.H13A_h	2.8647	C1	.H3B_e	3.0085
O1'	.H62'_g	2.6451	C3	.H31'	2.5950
O11	.H12B	2.2996	C3'	.H3A	2.6106
O11	.H13C_n	2.7802	C5	.H52'	2.6052
O11	.H13D_o	2.5739	C5'	.H5B	2.6203
O11'	.H12C_p	2.6547	C11	.H15D_n	2.8980
O11'	.H15A	2.6954	C12	.H13C_n	3.0856
O11'	.H16B_p	2.8903	C12	.H12B_o	2.9401
O11'	.H13B	2.6662	C13	.H12B_o	2.8308
C13	.H13A	2.5842	H5B	.H52'	1.9211
C13	.H12A_p	3.0772	H6B	.H15C_j	2.3861
C13'	.H13D	2.5963	H11	.O1'_m	1.7296
C13'	.H12A_p	2.8902	H11	.S1'_m	2.4711
C14	.H12A_p	2.9180	H12A	.C13_n	3.0772
C14'	.H12A_p	2.8353	H12A	.C13'_n	2.8902
C15	.H20_r	2.9643	H12A	.H13B_n	2.5494

C15	.H15B	2.5945	H12A	.C14'_n	2.8353
C15	.H16D_p	3.0988	H12A	.C14_n	2.9180
C15'	.H15C	2.6089	H12B	.H13C_o	2.5716
C15'	.H16D_p	2.9832	H12B	.H12B_o	2.2734
C16	.H15D_n	3.0848	H12B	.O11	2.2996
C21	.H61'_e	3.0925	H12B	.C13_o	2.8308
C22	.H51'_e	3.0223	H12B	.C12_o	2.9401
H1	.O11'_d	1.4824	H12C	.O11'_n	2.6547
H1	.S11'_d	2.5143	H13A	.O1'_s	2.8647
H2A	.O1	2.3485	H13A	.C13	2.5842
H2B	.H3A_f	2.5651	H13A	.H13D	1.8962
H3A	.H2B_f	2.5651	H13B	.O11'	2.6662
H3A	.C3'	2.6106	H13B	.H12A_p	2.5494
H3A	.H31'	1.9100	H13B	.H15A	2.5317
H3B	.N1_g	2.9014	H13C	.C12_p	3.0856
H3B	.H5A	2.5751	H13C	.O11_p	2.7802
H3B	.O1_g	2.6339	H13C	.H12B_o	2.5716
H3B	.C1_g	3.0085	H13C	.H15D	2.5536
H5A	.H3B	2.5751	H13D	.O11_o	2.5739
H5A	.N1_g	2.8744	H13D	.C13'	2.5963
H5B	.C5'	2.6203	H13D	.H13A	1.8962
H15A	.O11'	2.6954	H20	.H15D_j	2.4966
H15A	.H13B	2.5317	H20	.C15_j	2.9643
H15B	.C15	2.5945	H20	.H16C_j	2.4913
H15B	.H15C	1.9077	H21	.N11_u	2.6357
H15C	.H15B	1.9077	H21'	.O1'_e	2.7529
H15C	.H6B_f	2.3861	H22'	.O1_f	2.6876
H15C	.C15'	2.6089	H31'	.H3A	1.9100
H15D	.N11_p	2.7672	H31'	.C3	2.5950
H15D	.C16_p	3.0848	H32'	.O1'	2.6783
H15D	.C11_p	2.8980	H32'	.H51'	2.5603
H15D	.H20_r	2.4966	H51'	.O1'	2.6711
H15D	.H13C	2.5536	H51'	.C22_i	3.0223
H16A	.O11'_h	2.4338	H51'	.H32'	2.5603
H16B	.O11'_n	2.8903	H52'	.H5B	1.9211
H16C	.H20_r	2.4913	H52'	.C5	2.6052

H16D	.C15'_n	2.9832	H61'	.C21_i	3.0925
H16D	.C15_n	3.0988	H62'	.O1'_e	2.6451

Table S9 - Hydrogen Bonds (Angstrom, Deg)

O1 -- H1 .. S11'	1.2397	2.5143	3.696(5)	158.54	1_465	yes
O1 -- H1 .. O11'	1.2397	1.4824	2.706(6)	167.54	1_465	yes
O11 -- H11 .. S1'	1.1218	2.4711	3.540(5)	158.65	1_456	yes
O11 -- H11 .. O1'	1.1218	1.7296	2.729(6)	145.46	1_456	yes
C2 -- H2A .. O1	0.9710	2.3485	2.715(11)	101.52	.	yes
C12 -- H12B .. O11	0.9702	2.2996	2.704(8)	104.02	.	yes
C13 -- H13D .. O11	0.9699	2.5739	3.406(8)	143.89	2_657	yes
C16' -- H16A .. O11'	0.9705	2.4338	3.373(6)	162.65	2_756	yes

Translation of Symmetry Code to Equiv.Pos

a =[2565.00] = -x,1-y,-z
b =[1654.00] = 1+x,y,-1+z
c =[1565.00] = x,1+y,z
d =[1465.00] = -1+x,1+y,z
e =[1455.00] = -1+x,y,z
f =[2666.00] = 1-x,1-y,1-z
g =[1655.00] = 1+x,y,z
h =[2756.00] = 2-x,-y,1-z
i =[1655.00] = 1+x,y,z
j =[2666.00] = 1-x,1-y,1-z
k =[1545.00] = x,-1+y,z
l =[1645.00] = 1+x,-1+y,z
m =[1456.00] = -1+x,y,1+z
n =[1455.00] = -1+x,y,z
o =[2657.00] = 1-x,-y,2-z
p =[1655.00] = 1+x,y,z
q =[1556.00] = x,y,1+z
r =[2666.00] = 1-x,1-y,1-z
t =[2665.00] = 1-x,1-y,-z
u =[1554.00] = x,y,-1+z