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SUPPLEMENTARY MATERIAL FOR Lamellarin K triacetate (7)

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BELONGING TO THE PAPER

by

Contents

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Table S1 - Crystal Data and Details of the Structure Determination
for: compound 7

Crystal Data

Formula	C35 H31 N O12
Formula Weight	657.61
Crystal System	Monoclinic
Space group	P21/c (No. 14)
a, b, c [Angstrom]	10.5305(6) 12.3030(7) 24.7235(15)
alpha, beta, gamma [deg]	90 92.9450(10) 90
V [Ang**3]	3198.9(3)
Z	4
D(calc) [g/cm**3]	1.365
Mu(MoKa) [/mm]	0.104
F(000)	1376
Crystal Size [mm]	0.19 x 0.25 x 0.28

Data Collection

Temperature (K)	293
Radiation [Angstrom]	MoKa 0.71073
Theta Min-Max [Deg]	1.6, 28.0
Dataset	-13: 13 ; -15: 16 ; -32: 19
Tot., Uniq. Data, R(int)	19590, 7333, 0.029
Observed data [I > 2.0 sigma(I)]	3772

Refinement

Nref, Npar	7333, 440
R, wR2, S	0.0655, 0.2302, 1.04
w = 1/[\s^2^(Fo^2^)+(0.1273P)^2^+0.0791P] where P=(Fo^2^+2Fc^2^)/3	
Max. and Av. Shift/Error	0.00, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]	-0.24, 0.27

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: compound 7

Atom	x	y	z	U(eq) [Ang^2]
O1	0.4604(2)	1.20542(16)	0.90349(10)	0.0861(8)
O2	0.4658(2)	1.27603(16)	0.98553(10)	0.0932(9)
O3	0.22334(19)	0.98073(18)	1.21158(8)	0.0832(8)
O4	0.0585(3)	1.0866(2)	1.22609(11)	0.1127(11)
O5	0.0329(2)	0.83051(16)	1.20409(9)	0.0826(8)
O6	-0.0623(2)	0.75915(15)	1.10602(9)	0.0800(8)
O7	0.2165(2)	0.55431(14)	0.94179(10)	0.0872(8)
O8	0.01536(18)	0.57470(15)	0.87262(10)	0.0826(8)
O9	-0.1379(4)	0.5795(3)	0.92935(15)	0.1519(17)
O10	0.35457(19)	0.8946(2)	0.74661(9)	0.0862(8)
O11	0.4922(2)	1.0674(2)	0.72464(10)	0.0982(10)
O12	0.3241(3)	1.1612(3)	0.69295(14)	0.1572(17)
N1	0.3147(2)	1.08368(17)	1.02061(10)	0.0674(8)
C1	0.2436(2)	0.99050(19)	1.01642(12)	0.0591(9)
C2	0.1822(2)	0.9514(2)	1.06408(11)	0.0608(9)
C3	0.0851(2)	0.8738(2)	1.06056(12)	0.0630(9)
C4	0.0314(3)	0.8348(2)	1.10621(12)	0.0652(10)
C5	0.0744(3)	0.8729(2)	1.15781(12)	0.0663(10)
C6	0.1703(3)	0.9511(2)	1.16021(12)	0.0660(10)
C7	0.2235(2)	0.9931(2)	1.11520(12)	0.0618(9)
C8	0.3234(3)	1.0800(2)	1.11787(14)	0.0734(10)
C9	0.3237(3)	1.1483(2)	1.07025(13)	0.0879(11)
C10	0.3591(2)	1.10724(19)	0.97088(13)	0.0663(9)
C11	0.4312(3)	1.2009(2)	0.95647(15)	0.0748(10)
C12	0.4271(3)	1.1238(2)	0.86583(14)	0.0739(10)
C13	0.4690(3)	1.1381(3)	0.81500(15)	0.0850(13)

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms (continued) for: compound 7

Atom	x	y	z	U(eq) [Ang^2]
C14	0.4435(3)	1.0599(3)	0.77610(14)	0.0819(11)
C15	0.3742(3)	0.9660(2)	0.78767(13)	0.0717(10)
C16	0.3325(3)	0.9542(2)	0.83939(12)	0.0672(10)
C17	0.3564(2)	1.0333(2)	0.87954(13)	0.0643(9)
C18	0.3191(2)	1.02622(19)	0.93416(12)	0.0607(9)
C19	0.2462(2)	0.95204(18)	0.96314(11)	0.0574(8)
C20	0.1835(2)	0.85247(18)	0.94042(10)	0.0556(8)
C21	0.0785(2)	0.8605(2)	0.90506(12)	0.0661(9)
C22	0.0216(3)	0.7675(2)	0.88300(13)	0.0705(10)
C23	0.0695(2)	0.6679(2)	0.89681(12)	0.0656(9)
C24	0.1758(2)	0.65658(18)	0.93196(11)	0.0616(9)
C25	0.2318(2)	0.74945(18)	0.95367(11)	0.0572(8)
C26	-0.0895(4)	0.5368(3)	0.89171(18)	0.0931(16)
C27	-0.1409(4)	0.4428(3)	0.8611(2)	0.1164(18)
C28	0.3154(3)	0.5395(2)	0.98175(15)	0.0888(13)
C29	-0.0969(3)	0.7083(3)	1.05581(14)	0.0888(12)
C30	-0.0940(3)	0.8548(3)	1.21732(16)	0.1023(16)
C31	0.1577(3)	1.0493(3)	1.24235(15)	0.0851(14)
C32	0.2263(4)	1.0704(3)	1.29516(15)	0.1120(17)
C33	0.4222(4)	1.1175(4)	0.68503(17)	0.1065(16)
C34	0.4798(5)	1.1032(4)	0.63245(19)	0.145(2)
C35	0.2708(3)	0.8072(3)	0.75523(14)	0.0883(12)

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

Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters
for: compound 7

Atom	x	y	z	U(iso) [Ang^2]
H3	0.05630	0.84820	1.02670	0.0760
H8A	0.31070	1.12550	1.14920	0.0880
H8B	0.40620	1.04590	1.12310	0.0880
H9A	0.40140	1.19080	1.07120	0.1050
H9B	0.25260	1.19840	1.07040	0.1050
H13	0.51440	1.20020	0.80670	0.1020
H16	0.28740	0.89210	0.84790	0.0810
H20	0.04540	0.92860	0.89590	0.0790
H21	-0.04890	0.77320	0.85890	0.0850
H24	0.30280	0.74330	0.97750	0.0690
H26A	0.38720	0.58300	0.97310	0.1330
H26B	0.33970	0.46430	0.98300	0.1330
H26C	0.28660	0.56110	1.01640	0.1330
H27A	-0.12700	0.76220	1.03020	0.1330
H27B	-0.16290	0.65600	1.06100	0.1330
H27C	-0.02410	0.67220	1.04230	0.1330
H30A	-0.10600	0.93220	1.21740	0.1530
H30B	-0.10920	0.82630	1.25250	0.1530
H30C	-0.15240	0.82240	1.19090	0.1530
H31A	0.30620	1.10480	1.28920	0.1680
H31B	0.24130	1.00280	1.31390	0.1680
H31C	0.17600	1.11710	1.31660	0.1680
H32A	0.30600	0.76180	0.78380	0.1320
H32B	0.25940	0.76530	0.72260	0.1320
H32C	0.19010	0.83510	0.76520	0.1320
H33A	0.41630	1.11440	0.60370	0.2170

Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters (continued)
for: compound 7

Atom	x	y	z	U(iso) [Ang^2]
H33B	0.51340	1.03090	0.63010	0.2170
H33C	0.54720	1.15490	0.62920	0.2170
H37A	-0.18530	0.39620	0.88490	0.1750
H37B	-0.07250	0.40330	0.84610	0.1750
H37C	-0.19860	0.46750	0.83240	0.1750

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
for: compound 7

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
O1	0.0811(13)	0.0633(12)	0.1143(18)	0.0031(12)	0.0076(13)	-0.0250(10)
O2	0.0908(14)	0.0601(12)	0.1273(19)	-0.0075(12)	-0.0086(14)	-0.0249(11)
O3	0.0764(13)	0.0905(14)	0.0814(14)	-0.0140(11)	-0.0087(11)	0.0147(11)
O4	0.1114(19)	0.1109(19)	0.114(2)	-0.0196(15)	-0.0125(16)	0.0444(16)
O5	0.0810(13)	0.0832(14)	0.0837(14)	0.0096(12)	0.0063(11)	0.0144(11)
O6	0.0835(13)	0.0651(11)	0.0915(15)	0.0012(11)	0.0058(12)	-0.0182(10)
O7	0.0841(13)	0.0430(10)	0.1306(19)	-0.0074(10)	-0.0310(13)	0.0006(9)
O8	0.0635(12)	0.0602(11)	0.1224(18)	-0.0262(11)	-0.0121(12)	-0.0097(9)
O9	0.170(3)	0.138(3)	0.152(3)	-0.036(2)	0.050(3)	-0.087(2)
O10	0.0727(13)	0.1049(16)	0.0810(15)	-0.0037(13)	0.0039(11)	-0.0076(12)
O11	0.0730(13)	0.1260(19)	0.0960(17)	0.0306(14)	0.0091(13)	0.0043(13)
O12	0.133(3)	0.193(3)	0.147(3)	0.059(2)	0.021(2)	0.066(3)
N1	0.0672(14)	0.0509(12)	0.0829(17)	-0.0050(11)	-0.0077(12)	-0.0105(10)
C1	0.0543(14)	0.0418(12)	0.0798(19)	-0.0066(12)	-0.0089(13)	-0.0030(10)
C2	0.0588(15)	0.0490(13)	0.0736(18)	-0.0015(13)	-0.0068(13)	0.0039(11)
C3	0.0661(15)	0.0469(13)	0.0753(19)	-0.0064(13)	-0.0040(14)	-0.0042(12)
C4	0.0646(15)	0.0495(14)	0.081(2)	0.0006(14)	-0.0024(15)	0.0020(12)
C5	0.0687(16)	0.0575(15)	0.0723(19)	0.0043(14)	0.0006(15)	0.0123(13)
C6	0.0655(16)	0.0627(16)	0.0684(19)	-0.0096(14)	-0.0115(14)	0.0153(13)
C7	0.0571(14)	0.0484(13)	0.0786(19)	-0.0068(13)	-0.0098(14)	0.0081(11)
C8	0.0661(16)	0.0612(16)	0.091(2)	-0.0113(15)	-0.0144(15)	0.0003(13)
C9	0.100(2)	0.0683(19)	0.094(2)	-0.0216(18)	-0.0074(19)	-0.0251(17)
C10	0.0594(15)	0.0443(13)	0.094(2)	-0.0044(14)	-0.0080(15)	-0.0079(11)
C11	0.0661(17)	0.0553(16)	0.102(2)	0.0024(16)	-0.0046(16)	-0.0138(13)
C12	0.0628(16)	0.0615(16)	0.097(2)	0.0066(16)	0.0014(16)	-0.0102(13)
C13	0.0700(18)	0.078(2)	0.107(3)	0.018(2)	0.0047(19)	-0.0141(16)

Table S4 - (An)isotropic Displacement Parameters (continued)
for: compound 7

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
C14	0.0549(16)	0.104(2)	0.087(2)	0.020(2)	0.0050(16)	-0.0010(16)
C15	0.0515(14)	0.0819(19)	0.081(2)	0.0063(17)	-0.0027(14)	-0.0019(14)
C16	0.0531(14)	0.0667(16)	0.081(2)	0.0042(15)	-0.0040(14)	-0.0033(12)
C17	0.0486(13)	0.0576(15)	0.086(2)	0.0047(14)	-0.0043(13)	-0.0042(11)
C18	0.0524(14)	0.0477(13)	0.081(2)	-0.0012(13)	-0.0053(13)	-0.0027(11)
C19	0.0511(13)	0.0425(12)	0.0776(18)	0.0014(12)	-0.0062(12)	-0.0023(10)
C20	0.0508(13)	0.0446(12)	0.0712(17)	-0.0037(11)	0.0006(12)	-0.0054(10)
C21	0.0566(14)	0.0473(13)	0.093(2)	-0.0010(13)	-0.0092(14)	0.0035(11)
C22	0.0546(14)	0.0626(16)	0.092(2)	-0.0070(14)	-0.0172(14)	-0.0022(12)
C23	0.0535(14)	0.0511(14)	0.091(2)	-0.0152(14)	-0.0075(14)	-0.0062(11)
C24	0.0566(14)	0.0414(13)	0.0860(19)	-0.0040(12)	-0.0047(14)	-0.0011(10)
C25	0.0511(13)	0.0473(13)	0.0719(17)	-0.0019(12)	-0.0087(12)	-0.0003(10)
C26	0.101(3)	0.069(2)	0.108(3)	-0.009(2)	-0.007(2)	-0.0203(19)
C27	0.105(3)	0.0664(19)	0.173(4)	-0.018(2)	-0.038(3)	-0.0187(18)
C28	0.090(2)	0.0536(16)	0.120(3)	0.0098(16)	-0.023(2)	0.0006(15)
C29	0.089(2)	0.077(2)	0.099(2)	0.0020(18)	-0.0090(19)	-0.0244(17)
C30	0.082(2)	0.112(3)	0.114(3)	0.000(2)	0.017(2)	0.0127(19)
C31	0.083(2)	0.076(2)	0.096(3)	-0.0095(18)	0.0019(19)	0.0132(17)
C32	0.120(3)	0.129(3)	0.085(3)	-0.022(2)	-0.013(2)	0.015(2)
C33	0.088(2)	0.124(3)	0.108(3)	0.039(3)	0.010(2)	0.010(2)
C34	0.133(4)	0.196(5)	0.106(3)	0.057(3)	0.013(3)	0.021(4)
C35	0.078(2)	0.090(2)	0.096(2)	-0.0140(19)	-0.0035(18)	0.0042(18)

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)
for: compound 7

O1	-C11	1.362(4)	C4	-C5	1.412(4)
O1	-C12	1.402(4)	C5	-C6	1.394(4)
O2	-C11	1.215(4)	C6	-C7	1.372(4)
O3	-C6	1.409(4)	C7	-C8	1.499(4)
O3	-C31	1.350(4)	C8	-C9	1.447(4)
O4	-C31	1.192(4)	C10	-C11	1.435(4)
O5	-C5	1.350(4)	C10	-C18	1.399(4)
O5	-C30	1.424(4)	C12	-C13	1.365(5)
O6	-C4	1.356(3)	C12	-C17	1.391(4)
O6	-C29	1.421(4)	C13	-C14	1.377(5)
O7	-C24	1.347(3)	C14	-C15	1.404(4)
O7	-C28	1.410(4)	C15	-C16	1.381(4)
O8	-C23	1.401(3)	C16	-C17	1.404(4)
O8	-C26	1.309(5)	C17	-C18	1.428(4)
O9	-C26	1.204(6)	C18	-C19	1.411(3)
O10	-C15	1.350(4)	C19	-C20	1.488(3)
O10	-C35	1.414(4)	C20	-C21	1.377(3)
O11	-C14	1.399(4)	C20	-C25	1.398(3)
O11	-C33	1.345(5)	C21	-C22	1.390(4)
O12	-C33	1.190(5)	C22	-C23	1.362(4)
N1	-C1	1.370(3)	C23	-C24	1.388(3)
N1	-C9	1.461(4)	C24	-C25	1.382(3)
N1	-C10	1.369(4)	C26	-C27	1.470(6)
C1	-C2	1.455(4)	C31	-C32	1.482(5)
C1	-C19	1.401(4)	C33	-C34	1.473(6)
C2	-C3	1.398(3)	C3	-H3	0.9305
C2	-C7	1.412(4)	C8	-H8A	0.9705
C3	-C4	1.375(4)	C8	-H8B	0.9703

Table S5 - Bond Distances (Angstrom) (continued)
for: compound 7

C9	-H9A	0.9703	C29	-H27B	0.9606
C9	-H9B	0.9699	C29	-H27C	0.9606
C13	-H13	0.9298	C30	-H30A	0.9606
C16	-H16	0.9294	C30	-H30B	0.9588
C21	-H20	0.9309	C30	-H30C	0.9605
C22	-H21	0.9304	C32	-H31A	0.9599
C25	-H24	0.9309	C32	-H31B	0.9611
C27	-H37A	0.9601	C32	-H31C	0.9594
C27	-H37B	0.9591	C34	-H33A	0.9605
C27	-H37C	0.9595	C34	-H33B	0.9602
C28	-H26A	0.9594	C34	-H33C	0.9595
C28	-H26B	0.9600	C35	-H32A	0.9599
C28	-H26C	0.9608	C35	-H32B	0.9597
C29	-H27A	0.9594	C35	-H32C	0.9604

Table S6 - Bond Angles (Degrees)
for: compound 7

C11	-O1	-C12	123.3(2)	C2	-C7	-C8	118.8(2)
C6	-O3	-C31	118.6(2)	C6	-C7	-C8	123.2(3)
C5	-O5	-C30	117.5(3)	C7	-C8	-C9	114.2(3)
C4	-O6	-C29	117.3(2)	N1	-C9	-C8	111.4(2)
C24	-O7	-C28	117.6(2)	N1	-C10	-C11	127.1(3)
C23	-O8	-C26	118.0(3)	N1	-C10	-C18	109.1(2)
C15	-O10	-C35	117.0(2)	C11	-C10	-C18	123.8(3)
C14	-O11	-C33	118.7(3)	O1	-C11	-O2	117.5(3)
C1	-N1	-C9	122.0(2)	O1	-C11	-C10	114.8(3)
C1	-N1	-C10	108.7(2)	O2	-C11	-C10	127.6(3)
C9	-N1	-C10	129.0(2)	O1	-C12	-C13	116.0(3)
N1	-C1	-C2	118.6(2)	O1	-C12	-C17	122.0(3)
N1	-C1	-C19	108.5(2)	C13	-C12	-C17	122.0(3)
C2	-C1	-C19	132.9(2)	C12	-C13	-C14	119.5(3)
C1	-C2	-C3	122.0(2)	O11	-C14	-C13	121.4(3)
C1	-C2	-C7	118.4(2)	O11	-C14	-C15	117.3(3)
C3	-C2	-C7	119.6(2)	C13	-C14	-C15	121.2(3)
C2	-C3	-C4	121.2(3)	O10	-C15	-C14	116.3(3)
O6	-C4	-C3	124.5(3)	O10	-C15	-C16	125.7(2)
O6	-C4	-C5	115.5(3)	C14	-C15	-C16	117.9(3)
C3	-C4	-C5	120.0(3)	C15	-C16	-C17	121.9(2)
O5	-C5	-C4	122.3(2)	C12	-C17	-C16	117.5(3)
O5	-C5	-C6	119.7(3)	C12	-C17	-C18	117.1(3)
C4	-C5	-C6	117.8(3)	C16	-C17	-C18	125.3(2)
O3	-C6	-C5	118.0(3)	C10	-C18	-C17	118.8(2)
O3	-C6	-C7	118.3(2)	C10	-C18	-C19	106.6(2)
C5	-C6	-C7	123.4(3)	C17	-C18	-C19	134.6(2)
C2	-C7	-C6	118.0(2)	C1	-C19	-C18	107.2(2)

Table S6 - Bond Angles (Degrees) (continued)
for: compound 7

C1	-C19	-C20	127.1(2)	C9	-C8	-H8B	108.67
C18	-C19	-C20	125.7(2)	H8A	-C8	-H8B	107.62
C19	-C20	-C21	120.4(2)	N1	-C9	-H9A	109.37
C19	-C20	-C25	120.6(2)	N1	-C9	-H9B	109.40
C21	-C20	-C25	119.0(2)	C8	-C9	-H9A	109.29
C20	-C21	-C22	120.4(2)	C8	-C9	-H9B	109.39
C21	-C22	-C23	119.7(3)	H9A	-C9	-H9B	107.91
O8	-C23	-C22	119.5(2)	C12	-C13	-H13	120.23
O8	-C23	-C24	118.8(2)	C14	-C13	-H13	120.27
C22	-C23	-C24	121.6(2)	C15	-C16	-H16	119.12
O7	-C24	-C23	116.4(2)	C17	-C16	-H16	119.01
O7	-C24	-C25	125.2(2)	C20	-C21	-H20	119.82
C23	-C24	-C25	118.3(2)	C22	-C21	-H20	119.80
C20	-C25	-C24	121.0(2)	C21	-C22	-H21	120.19
O8	-C26	-O9	121.4(4)	C23	-C22	-H21	120.09
O8	-C26	-C27	112.9(4)	C20	-C25	-H24	119.51
O9	-C26	-C27	125.6(4)	C24	-C25	-H24	119.44
O3	-C31	-O4	121.1(3)	C26	-C27	-H37A	109.41
O3	-C31	-C32	111.4(3)	C26	-C27	-H37B	109.49
O4	-C31	-C32	127.5(3)	C26	-C27	-H37C	109.51
O11	-C33	-O12	122.4(4)	H37A	-C27	-H37B	109.48
O11	-C33	-C34	110.7(4)	H37A	-C27	-H37C	109.42
O12	-C33	-C34	126.8(4)	H37B	-C27	-H37C	109.52
C2	-C3	-H3	119.38	O7	-C28	-H26A	109.51
C4	-C3	-H3	119.45	O7	-C28	-H26B	109.46
C7	-C8	-H8A	108.75	O7	-C28	-H26C	109.47
C7	-C8	-H8B	108.74	H26A	-C28	-H26B	109.45
C9	-C8	-H8A	108.70	H26A	-C28	-H26C	109.45

Table S6 - Bond Angles (Degrees) (continued)
for: compound 7

H26B	-C28	-H26C	109.49	H31A	-C32	-H31B	109.38
O6	-C29	-H27A	109.48	H31A	-C32	-H31C	109.51
O6	-C29	-H27B	109.46	H31B	-C32	-H31C	109.49
O6	-C29	-H27C	109.51	C33	-C34	-H33A	109.47
H27A	-C29	-H27B	109.53	C33	-C34	-H33B	109.50
H27A	-C29	-H27C	109.43	C33	-C34	-H33C	109.55
H27B	-C29	-H27C	109.42	H33A	-C34	-H33B	109.44
O5	-C30	-H30A	109.49	H33A	-C34	-H33C	109.44
O5	-C30	-H30B	109.51	H33B	-C34	-H33C	109.43
O5	-C30	-H30C	109.41	O10	-C35	-H32A	109.46
H30A	-C30	-H30B	109.42	O10	-C35	-H32B	109.50
H30A	-C30	-H30C	109.46	O10	-C35	-H32C	109.51
H30B	-C30	-H30C	109.53	H32A	-C35	-H32B	109.45
C31	-C32	-H31A	109.47	H32A	-C35	-H32C	109.42
C31	-C32	-H31B	109.49	H32B	-C35	-H32C	109.49
C31	-C32	-H31C	109.49				

Table S7 - Torsion Angles (Degrees)
for: compound 7

C12	-O1	-C11	-C10	-2.1(4)
C11	-O1	-C12	-C13	-176.8(3)
C12	-O1	-C11	-O2	179.4(3)
C11	-O1	-C12	-C17	2.7(4)
C31	-O3	-C6	-C7	107.8(3)
C31	-O3	-C6	-C5	-78.0(3)
C6	-O3	-C31	-C32	179.2(3)
C6	-O3	-C31	-O4	-2.0(5)
C30	-O5	-C5	-C6	113.2(3)
C30	-O5	-C5	-C4	-72.0(4)
C29	-O6	-C4	-C5	-172.0(3)
C29	-O6	-C4	-C3	7.4(4)
C28	-O7	-C24	-C23	-173.2(3)
C28	-O7	-C24	-C25	7.3(4)
C23	-O8	-C26	-C27	176.7(3)
C26	-O8	-C23	-C22	-80.3(4)
C26	-O8	-C23	-C24	103.4(3)
C23	-O8	-C26	-O9	-0.8(5)
C35	-O10	-C15	-C16	8.5(4)
C35	-O10	-C15	-C14	-171.7(3)
C14	-O11	-C33	-O12	4.6(6)
C14	-O11	-C33	-C34	-171.6(3)
C33	-O11	-C14	-C15	92.5(4)
C33	-O11	-C14	-C13	-91.4(4)
C9	-N1	-C1	-C2	-4.1(3)
C9	-N1	-C1	-C19	175.6(2)
C10	-N1	-C1	-C2	-177.8(2)
C9	-N1	-C10	-C11	3.0(4)

Table S7 - Torsion Angles (Degrees) (continued)
for: compound 7

C9	-N1	-C10	-C18	-174.8(2)
C1	-N1	-C10	-C18	-1.7(3)
C1	-N1	-C9	-C8	35.6(4)
C10	-N1	-C1	-C19	1.9(3)
C10	-N1	-C9	-C8	-152.1(3)
C1	-N1	-C10	-C11	176.1(2)
N1	-C1	-C19	-C20	179.2(2)
C2	-C1	-C19	-C18	178.2(2)
C19	-C1	-C2	-C3	-15.1(4)
N1	-C1	-C19	-C18	-1.3(3)
N1	-C1	-C2	-C7	-16.1(3)
C2	-C1	-C19	-C20	-1.2(4)
C19	-C1	-C2	-C7	164.3(2)
N1	-C1	-C2	-C3	164.4(2)
C3	-C2	-C7	-C6	3.3(3)
C1	-C2	-C3	-C4	177.6(2)
C3	-C2	-C7	-C8	-177.2(2)
C7	-C2	-C3	-C4	-1.9(4)
C1	-C2	-C7	-C8	3.3(3)
C1	-C2	-C7	-C6	-176.2(2)
C2	-C3	-C4	-C5	-0.2(4)
C2	-C3	-C4	-O6	-179.5(2)
O6	-C4	-C5	-C6	-179.7(2)
C3	-C4	-C5	-C6	0.8(4)
C3	-C4	-C5	-O5	-174.1(2)
O6	-C4	-C5	-O5	5.4(4)
C4	-C5	-C6	-C7	0.6(4)
O5	-C5	-C6	-O3	1.9(4)

Table S7 - Torsion Angles (Degrees) (continued)
for: compound 7

C4	-C5	-C6	-O3	-173.2(2)
O5	-C5	-C6	-C7	175.7(2)
C5	-C6	-C7	-C8	177.8(3)
O3	-C6	-C7	-C2	171.1(2)
C5	-C6	-C7	-C2	-2.7(4)
O3	-C6	-C7	-C8	-8.4(4)
C2	-C7	-C8	-C9	28.7(3)
C6	-C7	-C8	-C9	-151.8(3)
C7	-C8	-C9	-N1	-46.1(3)
C18	-C10	-C11	-O2	177.5(3)
N1	-C10	-C11	-O1	-178.3(2)
C11	-C10	-C18	-C17	3.0(4)
N1	-C10	-C18	-C17	-179.0(2)
N1	-C10	-C18	-C19	0.9(3)
C18	-C10	-C11	-O1	-0.8(4)
C11	-C10	-C18	-C19	-177.1(2)
N1	-C10	-C11	-O2	-0.1(5)
O1	-C12	-C17	-C16	-177.5(3)
O1	-C12	-C17	-C18	-0.3(4)
C13	-C12	-C17	-C16	2.0(4)
C17	-C12	-C13	-C14	-1.5(5)
C13	-C12	-C17	-C18	179.2(3)
O1	-C12	-C13	-C14	178.1(3)
C12	-C13	-C14	-O11	-175.4(3)
C12	-C13	-C14	-C15	0.5(5)
O11	-C14	-C15	-O10	-3.9(4)
O11	-C14	-C15	-C16	175.9(3)
C13	-C14	-C15	-C16	-0.2(5)

Table S7 - Torsion Angles (Degrees) (continued)
for: compound 7

C13	-C14	-C15	-O10	180.0(3)
C14	-C15	-C16	-C17	0.7(4)
O10	-C15	-C16	-C17	-179.4(3)
C15	-C16	-C17	-C18	-178.6(3)
C15	-C16	-C17	-C12	-1.6(4)
C16	-C17	-C18	-C19	-5.3(4)
C12	-C17	-C18	-C10	-2.4(3)
C16	-C17	-C18	-C10	174.6(2)
C12	-C17	-C18	-C19	177.8(3)
C10	-C18	-C19	-C20	179.8(2)
C10	-C18	-C19	-C1	0.3(3)
C17	-C18	-C19	-C20	-0.4(4)
C17	-C18	-C19	-C1	-179.8(2)
C18	-C19	-C20	-C25	107.3(3)
C18	-C19	-C20	-C21	-71.3(3)
C1	-C19	-C20	-C21	108.0(3)
C1	-C19	-C20	-C25	-73.4(3)
C19	-C20	-C21	-C22	178.7(2)
C25	-C20	-C21	-C22	0.1(4)
C21	-C20	-C25	-C24	-0.1(4)
C19	-C20	-C25	-C24	-178.7(2)
C20	-C21	-C22	-C23	0.5(4)
C21	-C22	-C23	-O8	-177.2(3)
C21	-C22	-C23	-C24	-1.1(4)
C22	-C23	-C24	-C25	1.0(4)
O8	-C23	-C24	-O7	-2.4(4)
O8	-C23	-C24	-C25	177.1(2)
C22	-C23	-C24	-O7	-178.6(3)

Table S7 - Torsion Angles (Degrees) (continued)
for: compound 7

O7	-C24	-C25	-C20	179.1(2)
C23	-C24	-C25	-C20	-0.4(4)

Table S8 - Contact Distances(Angstrom)
for: compound 7

O2	.N1	3.004(3)	O2	.H9A	2.4886
O2	.C9	3.069(4)	O2	.H26B_a	2.6691
O2	.C28_b	3.305(4)	O2	.H24_b	2.5692
O3	.O5	2.726(3)	O3	.H8A	2.5579
O4	.O5	3.206(3)	O4	.H30A	2.5724
O4	.C5	3.134(4)	O4	.H32C_c	2.8081
O4	.C30	3.275(4)	O4	.H21_c	2.7164
O4	.C22_c	3.313(4)	O5	.H32B_d	2.6787
O5	.C35_d	3.228(4)	O6	.H31C_e	2.8954
O5	.O4	3.206(3)	O6	.H30C	2.4727
O5	.O6	2.721(3)	O6	.H37B_f	2.6904
O5	.C31	3.121(4)	O7	.H27B_f	2.6484
O5	.O3	2.726(3)	O9	.H26C_f	2.7311
O6	.C30	3.027(4)	O10	.H37C_g	2.6435
O6	.O5	2.721(3)	O12	.H37C_g	2.7809
O6	.C27_f	3.352(4)	O12	.H30B_c	2.6977
O7	.C26	3.399(5)	O12	.H8A_h	2.8392
O7	.O8	2.665(3)	N1	.O2	3.004(3)
O8	.O7	2.665(3)	C3	.C20	3.206(4)
O9	.C22	3.112(5)	C3	.C25	3.483(4)
O9	.C28_f	3.300(5)	C5	.O4	3.134(4)
O10	.C33	3.234(5)	C9	.O2	3.069(4)
O10	.O11	2.645(3)	C13	.O12	3.323(5)
O11	.O10	2.645(3)	C15	.O12	3.377(5)
O12	.C30_c	3.374(5)	C16	.C21	3.401(4)

O12	.C15	3.377(5)	C16	.C20	3.267(4)
O12	.C13	3.323(5)	C20	.C3	3.206(4)
O2	.H26A_b	2.5075	C20	.C16	3.267(4)

Table S8 - Contact Distances(Angstrom) (continued)
for: compound 7

C21	.C16	3.401(4)	C12	.H8B_b	2.7324
C22	.O9	3.112(5)	C13	.H8B_b	2.9979
C22	.O4_c	3.313(4)	C15	.H30A_c	3.0862
C25	.C3	3.483(4)	C16	.H32A	2.7442
C26	.O7	3.399(5)	C16	.H8B_b	2.8582
C27	.C35_i	3.539(6)	C16	.H30A_c	3.0446
C27	.O6_f	3.352(4)	C16	.H32C	2.7345
C28	.O9_f	3.300(5)	C17	.H8B_b	2.6870
C28	.O2_b	3.305(4)	C19	.H16	2.9961
C30	.O6	3.027(4)	C19	.H3	2.9023
C30	.O12_c	3.374(5)	C20	.H16	2.6314
C30	.O4	3.275(4)	C20	.H3	2.5770
C31	.O5	3.121(4)	C21	.H3	3.0322
C33	.O10	3.234(5)	C21	.H16	2.7031
C35	.O5_l	3.228(4)	C25	.H26A	2.6498
C35	.C27_g	3.539(6)	C25	.H26C	2.8313
C2	.H20_c	3.0243	C25	.H3	2.9145
C3	.H27A	2.6954	C26	.H21	3.0554
C3	.H20_c	3.0182	C28	.H24	2.5128
C3	.H27C	2.7613	C28	.H27B_f	3.0507
C4	.H20_c	3.0209	C29	.H3	2.4905
C4	.H30C	2.9275	C31	.H8A	3.0265
C5	.H32B_d	2.9885	C33	.H37C_g	3.0052
C5	.H20_c	3.0244	C34	.H9A_h	3.0446
C6	.H20_c	2.9918	C34	.H26A_j	3.0346

C7	.H20_c	2.9903	C35	.H16	2.5159
C10	.H27A_c	2.9237	C35	.H13_k	3.0902
C11	.H9A	2.8725	C35	.H37C_g	2.9987

Table S8 - Contact Distances(Angstrom) (continued)
for: compound 7

H3	.C19	2.9023	H20	.C5_c	3.0244
H3	.C20	2.5770	H20	.C6_c	2.9918
H3	.C21	3.0322	H20	.C7_c	2.9903
H3	.C25	2.9145	H21	.C26	3.0554
H3	.C29	2.4905	H21	.O4_c	2.7164
H3	.H27A	2.2068	H24	.C28	2.5128
H3	.H27C	2.3638	H24	.H26A	2.1682
H8A	.O3	2.5579	H24	.H26C	2.4486
H8A	.C31	3.0265	H24	.O2_b	2.5692
H8A	.O12_m	2.8392	H26A	.C25	2.6498
H8B	.C12_b	2.7324	H26A	.H24	2.1682
H8B	.C13_b	2.9979	H26A	.C34_k	3.0346
H8B	.C16_b	2.8582	H26A	.O2_b	2.5075
H8B	.C17_b	2.6870	H26B	.O2_n	2.6691
H9A	.O2	2.4886	H26B	.H27B_f	2.5753
H9A	.C11	2.8725	H26C	.C25	2.8313
H9A	.C34_m	3.0446	H26C	.H24	2.4486
H9A	.H33A_m	2.5300	H26C	.O9_f	2.7311
H13	.C35_j	3.0902	H27A	.C3	2.6954
H16	.C19	2.9961	H27A	.H3	2.2068
H16	.C20	2.6314	H27A	.C10_c	2.9237
H16	.C21	2.7031	H27B	.O7_f	2.6484
H16	.C35	2.5159	H27B	.C28_f	3.0507
H16	.H32A	2.2697	H27B	.H26B_f	2.5753
H16	.H32C	2.3467	H27C	.C3	2.7613

H20	.C2_c	3.0243	H27C	.H3	2.3638
H20	.C3_c	3.0182	H30A	.O4	2.5724
H20	.C4_c	3.0209	H30A	.C15_c	3.0862

Table S8 - Contact Distances(Angstrom) (continued)
for: compound 7

H30A	.C16_c	3.0446	H32B	.C5_l	2.9885
H30B	.O12_c	2.6977	H32C	.C16	2.7345
H30C	.O6	2.4727	H32C	.H16	2.3467
H30C	.C4	2.9275	H32C	.O4_c	2.8081
H30C	.H31C_e	2.5438	H33A	.H9A_h	2.5300
H31C	.O6_o	2.8954	H37B	.O6_f	2.6904
H31C	.H30C_o	2.5438	H37C	.O10_i	2.6435
H32A	.C16	2.7442	H37C	.O12_i	2.7809
H32A	.H16	2.2697	H37C	.C33_i	3.0052
H32B	.O5_l	2.6788	H37C	.C35_i	2.9987

Table S9 - Hydrogen Bonds (Angstrom, Deg)
for: compound 7

C9 -- H9A .. O2	0.9700	2.4900	3.069(4)	118.00	.
C25 -- H24 .. O2	0.9300	2.5700	3.465(3)	162.00	3_677
C28 -- H26A .. O2	0.9600	2.5100	3.305(4)	141.00	3_677
C30 -- H30A .. O4	0.9600	2.5700	3.275(4)	130.00	.
C30 -- H30C .. O6	0.9600	2.4700	3.027(4)	117.00	.

Translation of Symmetry Code to Equiv.Pos

a =[1565.00] = x,1+y,z
b =[3677.00] = 1-x,2-y,2-z
c =[3577.00] = -x,2-y,2-z
d =[4565.00] = x,3/2-y,1/2+z
e =[2547.00] = -x,-1/2+y,5/2-z
f =[3567.00] = -x,1-y,2-z
g =[2556.00] = -x,1/2+y,3/2-z
h =[4574.00] = x,5/2-y,-1/2+z
i =[2546.00] = -x,-1/2+y,3/2-z
j =[2656.00] = 1-x,1/2+y,3/2-z
k =[2646.00] = 1-x,-1/2+y,3/2-z
l =[4564.00] = x,3/2-y,-1/2+z
m =[4575.00] = x,5/2-y,1/2+z
n =[1545.00] = x,-1+y,z
o =[2557.00] = -x,1/2+y,5/2-z