Polymorph_2 P 21/c R = 0.06 : Nov 25 17:44:56 2021

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S U P P L E M E N T A R Y M A T E R I A L
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B E L O N G I N G T O T H E P A P E R

Portrayal of the Color Polymorphism in the 5-Acetyl-derivative of ROY

b y

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C o n t e n t s
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Table S1 - Crystal Data and Details of the Structure Determination
for: Polymorph_2 P 21/c R = 0.06

Crystal Data			
Formula			C13 H9 N3 O3 S
Formula Weight			287.29
Crystal System			monoclinic
Space group		P21/c	(No. 14)
a, b, c [Angstrom]	25.451(3)	14.4966(14)	7.1113(7)
alpha, beta, gamma [deg]	90	95.795(6)	90
V [Ang**3]			2610.3(5)
Z			8
D(calc) [g/cm**3]			1.462
Mu(MoKa) [/mm]			0.258
F(000)			1184
Crystal Size [mm]		0.12 x 0.30 x 0.50	

Data Collection			
Temperature (K)			296
Radiation [Angstrom]		MoKa	0.71073
Theta Min-Max [Deg]			2.4, 25.0
Dataset		-30: 30 ; -17: 17 ; -8: 8	
Tot., Uniq. Data, R(int)		207226, 4598, 0.116	
Observed Data [I > 2.0 sigma(I)]			3090

Refinement			
Nref, Npar			4598, 369
R, wR2, S		0.0584, 0.1582, 1.10	
w = ^2^(FO^2^)+(0.0545P)^2^+2.8905P] WHERE P=(FO^2^+2FC^2^)/3'			
Max. and Av. Shift/Error			0.00, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]			-0.26, 0.37

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms
for: Polymorph_2 P 21/c R = 0.06

Atom	x	y	z	U(eq) [Ang^2]
S1	0.28073(4)	0.23419(6)	0.46997(14)	0.0504(3)
S1'	0.22111(4)	0.54839(6)	0.55678(15)	0.0531(3)
O1	0.17683(12)	0.2918(2)	0.5654(5)	0.0850(14)
O2	0.44633(11)	0.03151(19)	0.3209(5)	0.0837(13)
O3	0.52147(12)	0.0849(2)	0.2718(6)	0.1015(16)
N1	0.33962(16)	-0.0984(3)	0.4818(7)	0.0866(18)
N2	0.37014(12)	0.1403(2)	0.3918(5)	0.0489(10)
N3	0.47593(13)	0.0970(2)	0.3038(5)	0.0611(12)
C1	0.32058(13)	0.1404(2)	0.4470(5)	0.0423(11)
O1'	0.32773(12)	0.4873(2)	0.4995(5)	0.0900(14)
C2	0.29533(14)	0.0595(2)	0.4902(5)	0.0508(12)
O2'	0.06262(12)	0.7555(2)	0.7402(6)	0.0910(13)
C3	0.24369(15)	0.0749(3)	0.5386(5)	0.0568(14)
O3'	-0.00855(14)	0.7023(3)	0.8329(7)	0.1259(19)
C4	0.23038(14)	0.1647(3)	0.5339(5)	0.0511(12)
C5	0.18106(15)	0.2083(3)	0.5716(6)	0.0600(16)
C6	0.13698(16)	0.1467(4)	0.6238(7)	0.086(2)
C7	0.31987(16)	-0.0286(3)	0.4854(6)	0.0591(14)
C8	0.40535(13)	0.2104(2)	0.3636(5)	0.0422(11)
C9	0.39223(14)	0.3036(2)	0.3754(5)	0.0481(12)
C10	0.42808(16)	0.3712(3)	0.3435(5)	0.0572(16)
C11	0.47814(16)	0.3497(3)	0.3013(6)	0.0613(16)

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms (continued)
for: Polymorph_2 P 21/c R = 0.06

Atom	x	y	z	U(eq) [Ang^2]
C12	0.49263(15)	0.2600(3)	0.2910(6)	0.0573(16)
C13	0.45695(13)	0.1904(2)	0.3209(5)	0.0464(12)
N1'	0.16577(15)	0.8814(2)	0.5760(6)	0.0756(16)
N2'	0.13069(12)	0.6453(2)	0.6115(5)	0.0509(10)
N3'	0.03323(13)	0.6901(2)	0.7673(6)	0.0735(14)
C1'	0.18208(12)	0.6437(2)	0.5748(5)	0.0401(11)
C2'	0.20986(13)	0.7238(2)	0.5519(5)	0.0453(11)
C3'	0.26276(14)	0.7080(3)	0.5205(5)	0.0517(12)
C4'	0.27500(14)	0.6176(3)	0.5184(5)	0.0526(14)
C5'	0.32506(16)	0.5709(3)	0.4996(6)	0.0665(16)
C6'	0.37239(16)	0.6318(4)	0.4814(9)	0.093(2)
C7'	0.18644(15)	0.8124(3)	0.5642(5)	0.0526(12)
C8'	0.09594(13)	0.5762(2)	0.6508(5)	0.0447(11)
C9'	0.10573(15)	0.4835(2)	0.6168(6)	0.0554(14)
C10'	0.07015(16)	0.4167(3)	0.6540(6)	0.0656(16)
C11'	0.02364(16)	0.4385(3)	0.7268(6)	0.0656(16)
C12'	0.01296(14)	0.5279(3)	0.7617(6)	0.0592(16)
C13'	0.04813(14)	0.5967(2)	0.7248(5)	0.0506(12)

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

Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters
for: Polymorph_2 P 21/c R = 0.06

Atom	x	y	z	U(iso) [Ang^2]
H2	0.3844(15)	0.090(3)	0.378(5)	0.0590
H3	0.22125	0.02805	0.57026	0.0680
H6A	0.10372	0.17088	0.56966	0.1290
H6B	0.13737	0.14448	0.75886	0.1290
H6C	0.14181	0.08570	0.57610	0.1290
H9	0.35875	0.32014	0.40519	0.0580
H10	0.41828	0.43279	0.35068	0.0680
H11	0.50190	0.39637	0.27993	0.0740
H12	0.52659	0.24510	0.26379	0.0690
H6A'	0.38462	0.65683	0.60295	0.1390
H2'	0.1207(15)	0.694(3)	0.636(6)	0.0610
H6B'	0.36260	0.68117	0.39502	0.1390
H3'	0.28673	0.75486	0.50304	0.0620
H6C'	0.40005	0.59602	0.43470	0.1390
H9'	0.13690	0.46665	0.56803	0.0670
H10'	0.07759	0.35535	0.62958	0.0780
H11'	-0.00010	0.39238	0.75173	0.0790
H12'	-0.01837	0.54326	0.81093	0.0710

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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

Table S4 - (An)isotropic Displacement Parameters
for: Polymorph_2 P 21/c R = 0.06

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
S1	0.0477(5)	0.0452(5)	0.0603(6)	0.0010(4)	0.0147(4)	0.0028(4)
S1'	0.0428(5)	0.0405(5)	0.0776(7)	0.0013(5)	0.0140(4)	0.0014(4)
O1	0.067(2)	0.074(2)	0.118(3)	0.007(2)	0.0294(18)	0.0187(17)
O2	0.0617(18)	0.0427(17)	0.152(3)	-0.0109(18)	0.0368(19)	0.0018(14)
O3	0.060(2)	0.072(2)	0.180(4)	0.015(2)	0.049(2)	0.0169(17)
N1	0.085(3)	0.047(2)	0.131(4)	0.003(2)	0.027(3)	0.002(2)
N2	0.0449(17)	0.0334(16)	0.070(2)	-0.0041(15)	0.0142(15)	0.0001(13)
N3	0.052(2)	0.054(2)	0.080(2)	0.0003(17)	0.0203(17)	0.0073(17)
C1	0.0463(19)	0.0383(19)	0.0427(19)	-0.0002(15)	0.0065(15)	-0.0027(16)
O1'	0.0604(19)	0.065(2)	0.149(3)	-0.010(2)	0.032(2)	0.0068(16)
C2	0.050(2)	0.042(2)	0.061(2)	-0.0038(17)	0.0080(18)	-0.0066(17)
O2'	0.0657(19)	0.0450(17)	0.169(3)	-0.0114(19)	0.045(2)	0.0032(15)
C3	0.052(2)	0.056(2)	0.064(3)	-0.0044(19)	0.0134(19)	-0.0128(19)
O3'	0.079(2)	0.075(2)	0.238(5)	-0.019(3)	0.086(3)	0.0070(19)
C4	0.043(2)	0.059(2)	0.052(2)	-0.0027(18)	0.0078(17)	-0.0053(17)
C5	0.044(2)	0.068(3)	0.069(3)	-0.006(2)	0.0104(19)	0.005(2)
C6	0.050(3)	0.103(4)	0.110(4)	-0.023(3)	0.029(3)	-0.007(2)
C7	0.057(2)	0.039(2)	0.083(3)	0.000(2)	0.016(2)	-0.0095(19)
C8	0.0446(19)	0.0375(19)	0.045(2)	-0.0014(15)	0.0069(15)	-0.0037(15)
C9	0.049(2)	0.042(2)	0.054(2)	-0.0040(17)	0.0087(17)	-0.0041(17)
C10	0.066(3)	0.039(2)	0.067(3)	0.0008(18)	0.009(2)	-0.0058(19)
C11	0.057(2)	0.053(3)	0.075(3)	0.003(2)	0.012(2)	-0.017(2)

Table S4 - (An)isotropic Displacement Parameters (continued)
for: Polymorph_2 P 21/c R = 0.06

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
C12	0.045(2)	0.060(3)	0.068(3)	0.003(2)	0.0116(18)	-0.0068(18)
C13	0.046(2)	0.042(2)	0.052(2)	-0.0008(16)	0.0094(16)	0.0028(16)
N1'	0.084(3)	0.042(2)	0.100(3)	-0.0002(19)	0.005(2)	0.0061(19)
N2'	0.0428(17)	0.0346(16)	0.077(2)	0.0005(16)	0.0149(15)	0.0010(14)
N3'	0.051(2)	0.052(2)	0.122(3)	-0.007(2)	0.031(2)	0.0052(17)
C1'	0.0366(17)	0.0385(19)	0.0459(19)	0.0006(15)	0.0071(15)	-0.0010(15)
C2'	0.047(2)	0.0384(19)	0.051(2)	0.0010(16)	0.0077(16)	-0.0023(16)
C3'	0.049(2)	0.047(2)	0.060(2)	-0.0006(18)	0.0104(17)	-0.0071(17)
C4'	0.0402(19)	0.051(2)	0.068(3)	-0.0054(18)	0.0126(17)	-0.0044(16)
C5'	0.049(2)	0.067(3)	0.086(3)	-0.006(2)	0.019(2)	0.003(2)
C6'	0.045(2)	0.090(4)	0.147(5)	-0.012(3)	0.030(3)	-0.008(2)
C7'	0.056(2)	0.042(2)	0.060(2)	0.0050(18)	0.0069(18)	-0.0067(19)
C8'	0.0383(18)	0.0365(19)	0.059(2)	0.0055(16)	0.0037(16)	0.0003(15)
C9'	0.046(2)	0.040(2)	0.082(3)	-0.0028(19)	0.0153(19)	0.0007(17)
C10'	0.065(3)	0.040(2)	0.093(3)	0.000(2)	0.014(2)	-0.005(2)
C11'	0.057(2)	0.048(3)	0.094(3)	0.004(2)	0.019(2)	-0.0118(19)
C12'	0.044(2)	0.059(3)	0.077(3)	0.004(2)	0.018(2)	-0.0043(18)
C13'	0.046(2)	0.040(2)	0.067(2)	-0.0010(18)	0.0111(18)	0.0030(17)

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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)
for: Polymorph_2 P 21/c R = 0.06

S1	-C1	1.714(3)	N2'	-C8'	1.383(4)
S1	-C4	1.727(4)	N2'	-C1'	1.360(4)
S1'	-C4'	1.743(4)	C3	-H3	0.9300
S1'	-C1'	1.714(3)	N3'	-C13'	1.446(4)
O1	-C5	1.216(5)	C6	-H6C	0.9600
O2	-N3	1.226(4)	C6	-H6B	0.9600
O3	-N3	1.216(5)	C6	-H6A	0.9600
N1	-C7	1.131(6)	C9	-H9	0.9300
N2	-C8	1.383(4)	C10	-H10	0.9300
N2	-C1	1.358(5)	C11	-H11	0.9300
N3	-C13	1.447(4)	C12	-H12	0.9300
C1	-C2	1.387(4)	C1'	-C2'	1.378(4)
O1'	-C5'	1.214(5)	C2'	-C3'	1.406(5)
C2	-C7	1.424(5)	C2'	-C7'	1.422(5)
N2	-H2	0.83(4)	N2'	-H2'	0.78(4)
C2	-C3	1.410(5)	C3'	-C4'	1.347(6)
O2'	-N3'	1.235(4)	C4'	-C5'	1.461(6)
C3	-C4	1.345(6)	C5'	-C6'	1.510(6)
O3'	-N3'	1.217(5)	C8'	-C13'	1.405(5)
C4	-C5	1.454(5)	C8'	-C9'	1.392(4)
C5	-C6	1.509(6)	C9'	-C10'	1.370(5)
C8	-C9	1.396(4)	C10'	-C11'	1.376(6)
C8	-C13	1.408(5)	C11'	-C12'	1.352(6)
C9	-C10	1.373(5)	C12'	-C13'	1.383(5)
C10	-C11	1.374(6)	C3'	-H3'	0.9300
C11	-C12	1.356(6)	C6'	-H6A'	0.9600
C12	-C13	1.388(5)	C6'	-H6B'	0.9600
N1'	-C7'	1.137(5)	C6'	-H6C'	0.9600

Table S5 - Bond Distances (Angstrom) (continued)
for: Polymorph_2 P 21/c R = 0.06

C9'	-H9'	0.9300	C11'	-H11'	0.9300
C10'	-H10'	0.9300	C12'	-H12'	0.9300

Table S6 - Bond Angles (Degrees)
for: Polymorph_2 P 21/c R = 0.06

C1	-S1	-C4	91.39(18)	C11	-C12	-C13	120.2(4)
C1'	-S1'	-C4'	91.08(17)	C8	-C13	-C12	121.5(3)
C1	-N2	-C8	132.5(3)	N3	-C13	-C12	116.0(3)
O2	-N3	-C13	120.2(3)	N3	-C13	-C8	122.5(3)
O3	-N3	-C13	118.9(3)	C1'	-N2'	-C8'	132.3(3)
O2	-N3	-O3	120.9(3)	C2	-C3	-H3	124.00
S1	-C1	-N2	127.2(2)	C4	-C3	-H3	124.00
N2	-C1	-C2	121.9(3)	O2'	-N3'	-C13'	120.7(3)
S1	-C1	-C2	111.0(3)	O3'	-N3'	-C13'	118.3(3)
C1	-C2	-C3	112.6(3)	O2'	-N3'	-O3'	121.0(4)
C3	-C2	-C7	124.8(3)	H6B	-C6	-H6C	110.00
C1	-N2	-H2	118(3)	C5	-C6	-H6B	109.00
C8	-N2	-H2	110(3)	H6A	-C6	-H6C	110.00
C1	-C2	-C7	122.6(3)	C5	-C6	-H6A	109.00
C2	-C3	-C4	112.7(3)	C5	-C6	-H6C	109.00
S1	-C4	-C3	112.3(3)	H6A	-C6	-H6B	109.00
S1	-C4	-C5	118.2(3)	C8	-C9	-H9	120.00
C3	-C4	-C5	129.5(4)	C10	-C9	-H9	120.00
C4	-C5	-C6	117.7(4)	C9	-C10	-H10	119.00
O1	-C5	-C6	122.2(4)	C11	-C10	-H10	119.00
O1	-C5	-C4	120.1(4)	C12	-C11	-H11	120.00
N1	-C7	-C2	179.6(4)	C10	-C11	-H11	120.00
C9	-C8	-C13	116.5(3)	C13	-C12	-H12	120.00
N2	-C8	-C13	120.8(3)	C11	-C12	-H12	120.00
N2	-C8	-C9	122.7(3)	S1'	-C1'	-N2'	127.2(2)
C8	-C9	-C10	120.9(3)	S1'	-C1'	-C2'	111.3(2)
C9	-C10	-C11	121.4(4)	N2'	-C1'	-C2'	121.6(3)
C10	-C11	-C12	119.5(4)	C1'	-C2'	-C3'	113.1(3)

Table S6 - Bond Angles (Degrees) (continued)
for: Polymorph_2 P 21/c R = 0.06

C1'	-C2'	-C7'	122.0(3)	C8'	-C13'	-C12'	121.3(3)
C3'	-C2'	-C7'	124.8(3)	N3'	-C13'	-C8'	122.1(3)
C1'	-N2'	-H2'	114(3)	N3'	-C13'	-C12'	116.6(3)
C8'	-N2'	-H2'	113(3)	C2'	-C3'	-H3'	124.00
C2'	-C3'	-C4'	112.7(3)	C4'	-C3'	-H3'	124.00
S1'	-C4'	-C5'	117.1(3)	C5'	-C6'	-H6A'	109.00
S1'	-C4'	-C3'	111.8(3)	C5'	-C6'	-H6B'	109.00
C3'	-C4'	-C5'	131.0(4)	C5'	-C6'	-H6C'	109.00
C4'	-C5'	-C6'	116.6(4)	H6A'	-C6'	-H6B'	110.00
O1'	-C5'	-C6'	122.6(4)	H6A'	-C6'	-H6C'	109.00
O1'	-C5'	-C4'	120.8(4)	H6B'	-C6'	-H6C'	109.00
N1'	-C7'	-C2'	177.0(4)	C8'	-C9'	-H9'	120.00
C9'	-C8'	-C13'	116.5(3)	C10'	-C9'	-H9'	119.00
N2'	-C8'	-C9'	122.3(3)	C9'	-C10'	-H10'	119.00
N2'	-C8'	-C13'	121.2(3)	C11'	-C10'	-H10'	119.00
C8'	-C9'	-C10'	121.0(4)	C10'	-C11'	-H11'	120.00
C9'	-C10'	-C11'	121.4(4)	C12'	-C11'	-H11'	120.00
C10'	-C11'	-C12'	119.1(4)	C11'	-C12'	-H12'	120.00
C11'	-C12'	-C13'	120.7(4)	C13'	-C12'	-H12'	120.00

Table S7 - Torsion Angles (Degrees)
for: Polymorph_2 P 21/c R = 0.06

C4	-S1	-C1	-N2	178.3(3)
C4	-S1	-C1	-C2	-0.8(3)
C1	-S1	-C4	-C3	0.5(3)
C1	-S1	-C4	-C5	-178.8(3)
C4'	-S1'	-C1'	-N2'	-178.3(4)
C4'	-S1'	-C1'	-C2'	0.0(3)
C1'	-S1'	-C4'	-C3'	0.2(3)
C1'	-S1'	-C4'	-C5'	177.2(3)
C1	-N2	-C8	-C13	174.4(4)
C1	-N2	-C8	-C9	-5.6(6)
C8	-N2	-C1	-S1	10.0(6)
C8	-N2	-C1	-C2	-171.1(4)
O2	-N3	-C13	-C12	-177.2(4)
O3	-N3	-C13	-C8	-178.0(4)
O3	-N3	-C13	-C12	2.6(5)
O2	-N3	-C13	-C8	2.2(6)
S1	-C1	-C2	-C3	0.9(4)
S1	-C1	-C2	-C7	-179.0(3)
N2	-C1	-C2	-C3	-178.2(3)
N2	-C1	-C2	-C7	1.9(6)
C7	-C2	-C3	-C4	179.3(4)
C1	-C2	-C3	-C4	-0.5(5)
C2	-C3	-C4	-S1	0.0(4)
C2	-C3	-C4	-C5	179.1(4)
C3	-C4	-C5	-C6	-0.2(6)
S1	-C4	-C5	-O1	-3.0(5)
S1	-C4	-C5	-C6	178.9(3)
C3	-C4	-C5	-O1	177.9(4)

Table S7 - Torsion Angles (Degrees) (continued)
for: Polymorph_2 P 21/c R = 0.06

C13	-C8	-C9	-C10	1.0(5)
N2	-C8	-C13	-N3	0.1(5)
N2	-C8	-C13	-C12	179.6(4)
N2	-C8	-C9	-C10	-179.0(3)
C9	-C8	-C13	-N3	-179.9(3)
C9	-C8	-C13	-C12	-0.4(5)
C8	-C9	-C10	-C11	-0.8(6)
C9	-C10	-C11	-C12	-0.1(6)
C10	-C11	-C12	-C13	0.7(6)
C11	-C12	-C13	-N3	179.0(4)
C11	-C12	-C13	-C8	-0.4(6)
C8'	-N2'	-C1'	-S1'	2.7(6)
C8'	-N2'	-C1'	-C2'	-175.5(4)
C1'	-N2'	-C8'	-C9'	-15.4(6)
C1'	-N2'	-C8'	-C13'	165.7(4)
O2'	-N3'	-C13'	-C8'	-0.3(6)
O2'	-N3'	-C13'	-C12'	179.3(4)
O3'	-N3'	-C13'	-C8'	-179.3(4)
O3'	-N3'	-C13'	-C12'	0.4(6)
S1'	-C1'	-C2'	-C3'	-0.2(4)
S1'	-C1'	-C2'	-C7'	-178.8(3)
N2'	-C1'	-C2'	-C3'	178.2(3)
N2'	-C1'	-C2'	-C7'	-0.4(6)
C1'	-C2'	-C3'	-C4'	0.4(5)
C7'	-C2'	-C3'	-C4'	178.9(3)
C2'	-C3'	-C4'	-S1'	-0.3(4)
C2'	-C3'	-C4'	-C5'	-176.8(4)
S1'	-C4'	-C5'	-O1'	4.3(5)

Table S7 - Torsion Angles (Degrees) (continued)
for: Polymorph_2 P 21/c R = 0.06

S1'	-C4'	-C5'	-C6'	-175.5(4)
C3'	-C4'	-C5'	-O1'	-179.4(4)
C3'	-C4'	-C5'	-C6'	0.9(7)
N2'	-C8'	-C9'	-C10'	-178.8(4)
C13'	-C8'	-C9'	-C10'	0.1(6)
N2'	-C8'	-C13'	-N3'	-1.3(6)
N2'	-C8'	-C13'	-C12'	179.1(4)
C9'	-C8'	-C13'	-N3'	179.7(4)
C9'	-C8'	-C13'	-C12'	0.1(5)
C8'	-C9'	-C10'	-C11'	-0.3(6)
C9'	-C10'	-C11'	-C12'	0.2(7)
C10'	-C11'	-C12'	-C13'	0.1(6)
C11'	-C12'	-C13'	-N3'	-179.9(4)
C11'	-C12'	-C13'	-C8'	-0.2(6)

Table S8 - Contact Distances(Angstrom)
for: Polymorph_2 P 21/c R = 0.06

S1	.O1	2.918(3)	O1	.H9'	2.7300
S1	.C3	2.560(4)	N1	.C5'_f	3.435(7)
S1	.C8	3.352(4)	O1	.H6B	2.7800
S1	.C9	3.147(4)	O1	.H6B_a	2.4800
S1	.C4_a	3.550(4)	N1	.C3'_e	3.448(6)
S1	.S1_a	3.5851(15)	O1	.H6A	2.5600
S1	.S1_b	3.5851(15)	O1'	.H6A'	2.9100
S1'	.C9'	3.153(4)	N1'	.C8'_l	3.405(5)
S1'	.C3'	2.569(4)	O1'	.H9	2.6600
S1'	.C8'	3.345(4)	O1'	.H10	2.7500
S1'	.O1'	2.922(3)	O1'	.H6C'	2.5000
S1	.H9	2.4300	O2	.H11_c	2.5100
S1'	.H9'	2.4600	N2	.C7	2.872(5)
O1	.C9'	3.356(4)	N2	.N3	2.894(5)
O1	.S1	2.918(3)	N2	.C10_b	3.401(5)
O1	.C6_a	3.323(6)	N2	.O2	2.588(4)
O1	.C10'	3.375(5)	O2	.H2	1.87(4)
O1'	.C9	3.295(4)	N2'	.C7'	2.844(5)
O1'	.C10	3.340(5)	N2'	.N3'	2.891(5)
O1'	.S1'	2.922(3)	O2'	.H2'	1.94(4)
O2	.N2	2.588(4)	N2'	.O2'	2.591(4)
O2	.C8	2.823(4)	N2'	.C7'_m	3.440(5)
O2'	.C8'	2.826(4)	O2'	.H11'_i	2.5500
O2'	.N2'	2.591(4)	O3	.H11_c	2.8100
O3	.C12	2.650(5)	O3	.H12	2.3300
O3'	.C6_j	3.411(6)	N3	.C10_a	3.407(5)
O3'	.C12'	2.647(6)	O3	.H10_c	2.8700
O1	.H10'	2.7700	N3	.N2	2.894(5)

Table S8 - Contact Distances(Angstrom) (continued)
for: Polymorph_2 P 21/c R = 0.06

O3	.H6C'_d	2.6000	C4	.S1_b	3.550(4)
N3'	.N2'	2.891(5)	C4	.C2	2.293(5)
O3'	.H10'_i	2.8600	C4'	.C2'	2.292(5)
O3'	.H6A_j	2.6300	C5'	.N1_b	3.435(7)
O3'	.H11'_i	2.8300	C5'	.C7_b	3.524(6)
O3'	.H12'	2.3200	C6	.O1_b	3.323(6)
N1	.H3'_e	2.5300	C6	.O3'_g	3.411(6)
C1	.C3	2.327(5)	C6	.C3	3.026(6)
C1	.C9	3.061(4)	C6'	.C3'	3.040(6)
C1	.C9_b	3.485(5)	C7	.C5'_f	3.524(6)
C1'	.C7'_m	3.529(5)	C7	.N2	2.872(5)
C1'	.C9'	3.062(4)	C7'	.N2'	2.844(5)
N1'	.H3_k	2.5500	C7'	.C2'_m	3.499(5)
C1'	.C3'	2.323(5)	C7'	.C1'_l	3.529(5)
N2	.H9	2.6300	C7'	.N2'_l	3.440(5)
C2	.C4	2.293(5)	C8	.C11	2.806(5)
C2'	.C7'_l	3.499(5)	C8	.S1	3.352(4)
C2'	.C4'	2.292(5)	C8	.O2	2.823(4)
N2'	.H9'	2.6100	C8	.C11_b	3.566(5)
C3	.C6	3.026(6)	C8	.C9_a	3.460(5)
C3	.S1	2.560(4)	C8'	.C11'	2.804(5)
N3	.H12	2.5400	C8'	.O2'	2.826(4)
N3	.H2	2.44(4)	C8'	.S1'	3.345(4)
C3'	.N1_k	3.448(6)	C8'	.N1'_m	3.405(5)
N3'	.H12'	2.5400	C9	.C12	2.757(5)
C3'	.S1'	2.569(4)	C9	.O1'	3.295(4)
N3'	.H2'	2.50(4)	C9	.S1	3.147(4)
C3'	.C6'	3.040(6)	C9	.C1_a	3.485(5)

Table S8 - Contact Distances(Angstrom) (continued)
for: Polymorph_2 P 21/c R = 0.06

C9	.C1	3.061(4)	C12'	.C10'_n	3.549(6)
C9	.C13_b	3.421(5)	C12'	.O3'	2.647(6)
C9	.C8_b	3.460(5)	C13	.C12_b	3.450(6)
C9'	.C12'	2.746(5)	C13	.C10	2.731(5)
C9'	.C1'	3.062(4)	C13	.C10_a	3.516(5)
C9'	.S1'	3.153(4)	C13	.C9_a	3.421(5)
C9'	.O1	3.356(4)	C13	.C11_b	3.454(6)
C10	.N2_a	3.401(5)	C13'	.C10'	2.726(5)
C10	.C13_b	3.516(5)	C13'	.C11'_n	3.567(6)
C10	.N3_b	3.407(5)	C1	.H9	2.8100
C10	.C13	2.731(5)	C1'	.H9'	2.8100
C10	.O1'	3.340(5)	C2	.H2	2.52(4)
C10'	.C12'_n	3.549(6)	C2'	.H2'	2.44(4)
C10'	.C13'	2.726(5)	C3	.H6C	2.6400
C10'	.O1	3.375(5)	C3'	.H6B'	2.8000
C11	.C8_a	3.566(5)	C4	.H6C	2.5700
C11	.C8	2.806(5)	C4	.H6B	3.0000
C11	.C13_a	3.454(6)	C4'	.H6A'	2.8500
C11'	.C8'	2.804(5)	C4'	.H6B'	2.6400
C11'	.C12'_n	3.538(6)	C5	.H3	2.8100
C11'	.C13'_n	3.567(6)	C5'	.H3'	2.8400
C12	.C12_a	3.568(6)	C6	.H3	2.8100
C12	.C12_b	3.568(6)	C6'	.H3'	2.8300
C12	.C13_a	3.450(6)	C7	.H2	2.55(4)
C12	.C9	2.757(5)	C7	.H3	2.7600
C12	.O3	2.650(5)	C7'	.H3'	2.7600
C12'	.C9'	2.746(5)	C7'	.H2'	2.49(4)
C12'	.C11'_n	3.538(6)	C9'	.H2'	3.08(4)

Table S8 - Contact Distances(Angstrom) (continued)
for: Polymorph_2 P 21/c R = 0.06

C13	.H2	2.42(4)	H6C'	.O1'	2.5000
C13'	.H2'	2.46(4)	H6C'	.H10	2.5000
H6A'	.C4'	2.8500	H6C'	.O3_h	2.6000
H6A'	.O1'	2.9100	H6A	.O3'_g	2.6300
H2	.O2	1.87(4)	H6A	.O1	2.5600
H2	.N3	2.44(4)	H6B	.O1	2.7800
H2	.C2	2.52(4)	H6B	.C4	3.0000
H2	.C7	2.55(4)	H6B	.O1_b	2.4800
H2	.C13	2.42(4)	H6C	.C3	2.6400
H2'	.N3'	2.50(4)	H6C	.H3	2.1900
H2'	.C2'	2.44(4)	H6C	.C4	2.5700
H2'	.O2'	1.94(4)	H9	.S1	2.4300
H2'	.C9'	3.08(4)	H9	.O1'	2.6600
H2'	.C13'	2.46(4)	H9	.H10	2.2900
H2'	.C7'	2.49(4)	H9	.N2	2.6300
H6B'	.C4'	2.6400	H9	.C1	2.8100
H6B'	.H3'	2.4000	H9'	.S1'	2.4600
H6B'	.C3'	2.8000	H9'	.O1	2.7300
H3	.C6	2.8100	H9'	.N2'	2.6100
H3	.H6C	2.1900	H9'	.C1'	2.8100
H3	.C5	2.8100	H9'	.H10'	2.2800
H3	.C7	2.7600	H10	.O1'	2.7500
H3	.N1'_e	2.5500	H10	.H9	2.2900
H3'	.C7'	2.7600	H10	.H11	2.3000
H3'	.N1_k	2.5300	H10	.H6C'	2.5000
H3'	.C5'	2.8400	H10	.O3_h	2.8700
H3'	.C6'	2.8300	H10'	.H9'	2.2800
H3'	.H6B'	2.4000	H10'	.H11'	2.3000

Table S8 - Contact Distances(Angstrom) (continued)
for: Polymorph_2 P 21/c R = 0.06

H10'	.O1	2.7700	H11'	.O2'_g	2.5500
H10'	.O3'_g	2.8600	H11'	.O3'_g	2.8300
H11	.H10	2.3000	H12	.H11	2.2900
H11	.H12	2.2900	H12	.O3	2.3300
H11	.O3_h	2.8100	H12	.N3	2.5400
H11	.O2_h	2.5100	H12'	.O3'	2.3200
H11'	.H12'	2.2800	H12'	.N3'	2.5400
H11'	.H10'	2.3000	H12'	.H11'	2.2800

Table S9 - Hydrogen Bonds (Angstrom, Deg)
for: Polymorph_2 P 21/c R = 0.06

N2	-- H2	.. O2	0.83(4)	1.87(4)	2.588(4)	145(4)	.
N2	-- H2	.. N3	0.83(4)	2.44(4)	2.894(5)	116(3)	.
N2'	-- H2'	.. O2'	0.78(4)	1.94(4)	2.591(4)	142(4)	.
N2'	-- H2'	.. N3'	0.78(4)	2.50(4)	2.891(5)	113(3)	.
C3	-- H3	.. N1'	0.9300	2.5500	3.461(5)	165.00	1_545
C3'	-- H3'	.. N1	0.9300	2.5300	3.448(6)	169.00	1_565
C6	-- H6B	.. O1	0.9600	2.4800	3.323(6)	146.00	4_555
C9	-- H9	.. S1	0.9300	2.4300	3.147(4)	134.00	.
C9'	-- H9'	.. S1'	0.9300	2.4600	3.153(4)	132.00	.
C11	-- H11	.. O2	0.9300	2.5100	3.426(5)	170.00	2_655
C11'	-- H11'	.. O2'	0.9300	2.5500	3.467(5)	170.00	2_546
C12	-- H12	.. O3	0.9300	2.3300	2.650(5)	100.00	.
C12'	-- H12'	.. O3'	0.9300	2.3200	2.647(6)	100.00	.

Translation of Symmetry Code to Equiv.Pos

a =[4554.00] = [4_565] = x,1/2-y,-1/2+z
b =[4555.00] = [4_566] = x,1/2-y,1/2+z
c =[2645.00] = [2_645] = 1-x,-1/2+y,1/2-z
d =[2645.00] = [2_645] = 1-x,-1/2+y,1/2-z
e =[1545.00] = [1_545] = x,-1+y,z
f =[4554.00] = [4_565] = x,1/2-y,-1/2+z
g =[2546.00] = [2_546] = -x,-1/2+y,3/2-z
h =[2655.00] = [2_655] = 1-x,1/2+y,1/2-z
i =[2556.00] = [2_556] = -x,1/2+y,3/2-z
j =[2556.00] = [2_556] = -x,1/2+y,3/2-z
k =[1565.00] = [1_565] = x,1+y,z
l =[4564.00] = [4_575] = x,3/2-y,-1/2+z
m =[4565.00] = [4_576] = x,3/2-y,1/2+z
n =[3566.00] = [3_566] = -x,1-y,1-z