Polymorph_1 P 21/n R = 0.04 : Nov 25 17:45:36 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_1 P 21/n R = 0.04

Crystal Data			
Formula			C13 H9 N3 O3 S
Formula Weight			287.29
Crystal System			monoclinic
Space group		P21/n	(No. 14)
a, b, c [Angstrom]	5.3354(2)	14.2344(4)	17.1709(6)
alpha, beta, gamma [deg]	90	96.567(2)	90
V [Ang**3]			1295.51(8)
Z			4
D(calc) [g/cm**3]			1.473
Mu(MoKa) [/mm]			0.260
F(000)			592
Crystal Size [mm]		0.22 x 0.25 x 0.32	
Data Collection			
Temperature (K)			295
Radiation [Angstrom]		MoKa	0.71073
Theta Min-Max [Deg]			3.7, 27.5
Dataset		-6: 6 ; -18: 18 ; -22: 22	
Tot., Uniq. Data, R(int)		122630, 2963, 0.048	
Observed Data [I > 2.0 sigma(I)]			2292
Refinement			
Nref, Npar			2963, 185
R, wR2, S		0.0417, 0.1181, 1.06	
w = ^2^(FO^2^)+(0.0479P)^2^+0.5373P] WHERE P=(FO^2^+2FC^2^)/3'			
Max. and Av. Shift/Error			0.00, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]			-0.19, 0.27

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms
for: Polymorph_1 P 21/n R = 0.04

Atom	x	y	z	U(eq) [Ang^2]
S1	0.26654(9)	0.31751(4)	0.62894(3)	0.0546(2)
O1	0.2270(3)	0.13653(12)	0.54883(11)	0.0855(7)
O2	0.2298(5)	0.68077(12)	0.69017(13)	0.0956(8)
O3	0.5820(5)	0.74409(14)	0.72987(15)	0.1225(10)
N1	-0.3475(4)	0.58318(16)	0.57544(12)	0.0775(8)
N2	0.2116(3)	0.49757(12)	0.68237(11)	0.0582(6)
N3	0.4452(5)	0.67624(14)	0.72343(14)	0.0794(8)
C1	0.1233(3)	0.42463(13)	0.63616(11)	0.0489(6)
C2	-0.0963(3)	0.42995(14)	0.58427(11)	0.0515(6)
C3	-0.1478(3)	0.34707(15)	0.54116(11)	0.0541(6)
C4	0.0278(3)	0.27980(15)	0.55846(11)	0.0514(6)
C5	0.0441(4)	0.18453(16)	0.52840(12)	0.0594(7)
C6	-0.1718(4)	0.14869(19)	0.47313(14)	0.0746(8)
C7	-0.2411(4)	0.51390(17)	0.57805(11)	0.0589(7)
C8	0.4198(4)	0.50297(14)	0.73829(11)	0.0516(6)
C9	0.5224(4)	0.42408(15)	0.77671(13)	0.0655(7)
C10	0.7317(5)	0.43047(18)	0.83137(14)	0.0782(9)
C11	0.8461(5)	0.5145(2)	0.84986(16)	0.0808(10)
C12	0.7483(5)	0.59369(19)	0.81343(15)	0.0746(9)
C13	0.5372(4)	0.58883(14)	0.75890(12)	0.0589(7)

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

Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters
for: Polymorph_1 P 21/n R = 0.04

Atom	x	y	z	U(iso) [Ang^2]
H2	0.144(5)	0.549(2)	0.6757(16)	0.0870
H3	-0.28856	0.33932	0.50445	0.0650
H6A	-0.13972	0.08482	0.45933	0.1120
H6B	-0.19032	0.18674	0.42666	0.1120
H6C	-0.32404	0.15154	0.49793	0.1120
H9	0.44865	0.36571	0.76544	0.0790
H10	0.79652	0.37621	0.85625	0.0940
H11	0.98818	0.51773	0.88660	0.0970
H12	0.82433	0.65149	0.82541	0.0900

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_1 P 21/n R = 0.04

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
S1	0.0420(3)	0.0585(3)	0.0591(3)	0.0035(2)	-0.0117(2)	0.0035(2)
O1	0.0699(10)	0.0791(11)	0.0993(13)	-0.0135(10)	-0.0252(9)	0.0208(9)
O2	0.1230(17)	0.0575(10)	0.1032(15)	0.0050(9)	0.0000(13)	0.0209(11)
O3	0.166(2)	0.0610(11)	0.143(2)	0.0001(12)	0.0283(17)	-0.0357(13)
N1	0.0721(12)	0.0905(15)	0.0669(12)	0.0008(10)	-0.0052(9)	0.0325(11)
N2	0.0573(10)	0.0508(9)	0.0636(10)	0.0059(8)	-0.0061(8)	0.0050(8)
N3	0.1103(18)	0.0513(11)	0.0794(14)	-0.0054(10)	0.0226(13)	-0.0043(12)
C1	0.0427(9)	0.0554(11)	0.0474(9)	0.0083(8)	0.0005(7)	-0.0003(8)
C2	0.0405(9)	0.0661(12)	0.0472(10)	0.0113(9)	0.0022(7)	0.0096(8)
C3	0.0390(9)	0.0761(13)	0.0453(10)	0.0027(9)	-0.0038(7)	0.0042(9)
C4	0.0381(9)	0.0671(12)	0.0467(10)	0.0045(9)	-0.0045(7)	0.0013(8)
C5	0.0527(11)	0.0688(13)	0.0541(11)	-0.0010(10)	-0.0047(9)	0.0041(10)
C6	0.0672(14)	0.0835(16)	0.0680(14)	-0.0128(12)	-0.0148(11)	0.0003(12)
C7	0.0484(10)	0.0798(14)	0.0468(10)	0.0043(10)	-0.0024(8)	0.0137(10)
C8	0.0504(10)	0.0529(10)	0.0509(10)	-0.0019(8)	0.0030(8)	-0.0002(8)
C9	0.0783(14)	0.0543(12)	0.0583(12)	-0.0021(9)	-0.0167(10)	0.0002(10)
C10	0.0872(17)	0.0742(15)	0.0662(14)	-0.0146(12)	-0.0217(12)	0.0190(13)
C11	0.0654(14)	0.0923(19)	0.0790(16)	-0.0284(14)	-0.0159(12)	0.0044(13)
C12	0.0709(14)	0.0785(16)	0.0749(15)	-0.0269(13)	0.0101(12)	-0.0196(12)
C13	0.0662(12)	0.0535(11)	0.0584(11)	-0.0058(9)	0.0137(10)	-0.0032(9)

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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_1 P 21/n R = 0.04

S1	-C1	1.7164(19)	C5	-C6	1.496(3)
S1	-C4	1.7386(19)	C8	-C13	1.400(3)
O1	-C5	1.210(3)	C8	-C9	1.383(3)
O2	-N3	1.225(4)	C9	-C10	1.377(3)
O3	-N3	1.208(3)	C10	-C11	1.364(4)
N1	-C7	1.136(3)	C11	-C12	1.364(4)
N2	-C1	1.358(3)	C12	-C13	1.382(3)
N2	-C8	1.385(3)	C3	-H3	0.9300
N3	-C13	1.446(3)	C6	-H6A	0.9600
C1	-C2	1.391(2)	C6	-H6B	0.9600
C2	-C3	1.403(3)	C6	-H6C	0.9600
C2	-C7	1.420(3)	C9	-H9	0.9300
N2	-H2	0.82(3)	C10	-H10	0.9300
C3	-C4	1.349(3)	C11	-H11	0.9300
C4	-C5	1.457(3)	C12	-H12	0.9300

Table S6 - Bond Angles (Degrees)
for: Polymorph_1 P 21/n R = 0.04

C1	-S1	-C4	91.59(9)	C8	-C9	-C10	121.2(2)
C1	-N2	-C8	130.15(17)	C9	-C10	-C11	121.5(2)
O2	-N3	-O3	121.7(2)	C10	-C11	-C12	118.7(2)
O2	-N3	-C13	119.8(2)	C11	-C12	-C13	120.6(2)
O3	-N3	-C13	118.5(2)	C8	-C13	-C12	121.4(2)
S1	-C1	-N2	126.43(14)	N3	-C13	-C8	121.60(19)
S1	-C1	-C2	110.59(14)	N3	-C13	-C12	117.0(2)
N2	-C1	-C2	122.91(17)	C2	-C3	-H3	123.00
C1	-C2	-C3	113.08(17)	C4	-C3	-H3	123.00
C1	-C2	-C7	120.35(18)	C5	-C6	-H6A	109.00
C3	-C2	-C7	126.56(17)	C5	-C6	-H6B	109.00
C1	-N2	-H2	119.0(19)	C5	-C6	-H6C	109.00
C8	-N2	-H2	110.7(19)	H6A	-C6	-H6B	109.00
C2	-C3	-C4	113.05(16)	H6A	-C6	-H6C	109.00
S1	-C4	-C5	117.73(14)	H6B	-C6	-H6C	109.00
S1	-C4	-C3	111.67(16)	C8	-C9	-H9	119.00
C3	-C4	-C5	130.60(18)	C10	-C9	-H9	119.00
C4	-C5	-C6	117.99(19)	C9	-C10	-H10	119.00
O1	-C5	-C6	121.9(2)	C11	-C10	-H10	119.00
O1	-C5	-C4	120.11(19)	C10	-C11	-H11	121.00
N1	-C7	-C2	176.6(2)	C12	-C11	-H11	121.00
C9	-C8	-C13	116.54(19)	C11	-C12	-H12	120.00
N2	-C8	-C9	121.87(19)	C13	-C12	-H12	120.00
N2	-C8	-C13	121.59(18)				

Table S7 - Torsion Angles (Degrees)
for: Polymorph_1 P 21/n R = 0.04

C4	-S1	-C1	-N2	-178.33(18)
C4	-S1	-C1	-C2	-1.38(14)
C1	-S1	-C4	-C3	1.05(15)
C1	-S1	-C4	-C5	-178.53(16)
C8	-N2	-C1	-S1	-5.7(3)
C8	-N2	-C1	-C2	177.67(19)
C1	-N2	-C8	-C9	-24.6(3)
C1	-N2	-C8	-C13	155.5(2)
O2	-N3	-C13	-C8	18.6(4)
O2	-N3	-C13	-C12	-162.2(2)
O3	-N3	-C13	-C8	-163.9(2)
O3	-N3	-C13	-C12	15.4(3)
S1	-C1	-C2	-C3	1.4(2)
S1	-C1	-C2	-C7	-177.61(15)
N2	-C1	-C2	-C3	178.48(17)
N2	-C1	-C2	-C7	-0.5(3)
C1	-C2	-C3	-C4	-0.6(2)
C7	-C2	-C3	-C4	178.31(18)
C2	-C3	-C4	-S1	-0.4(2)
C2	-C3	-C4	-C5	179.07(19)
S1	-C4	-C5	-O1	-4.6(3)
S1	-C4	-C5	-C6	174.67(15)
C3	-C4	-C5	-O1	176.0(2)
C3	-C4	-C5	-C6	-4.8(3)
N2	-C8	-C9	-C10	179.1(2)
C13	-C8	-C9	-C10	-1.0(3)
N2	-C8	-C13	-N3	0.7(3)
N2	-C8	-C13	-C12	-178.5(2)

Table S7 - Torsion Angles (Degrees) (continued)
for: Polymorph_1 P 21/n R = 0.04

C9	-C8	-C13	-N3	-179.3(2)
C9	-C8	-C13	-C12	1.6(3)
C8	-C9	-C10	-C11	0.0(4)
C9	-C10	-C11	-C12	0.5(4)
C10	-C11	-C12	-C13	0.1(4)
C11	-C12	-C13	-N3	179.7(2)
C11	-C12	-C13	-C8	-1.1(4)

Table S8 - Contact Distances(Angstrom)
for: Polymorph_1 P 21/n R = 0.04

S1	.O1	2.9166(18)	N2	.N3	2.884(3)
S1	.C3	2.5639(18)	O3	.H12	2.3700
S1	.C3_a	3.6456(17)	O3	.H10_f	2.5200
S1	.C8	3.288(2)	N3	.N2	2.884(3)
S1	.C9	3.132(2)	N3	.N1_a	3.175(3)
S1	.O3_b	3.385(3)	N3	.S1_e	3.522(2)
S1	.N3_b	3.522(2)	C1	.C3	2.331(3)
S1	.H9	2.5300	C1	.N1	3.448(3)
O1	.S1	2.9166(18)	N1	.H3_h	2.5000
O1	.C11_c	3.213(3)	C1	.C9	3.030(3)
O2	.N2	2.612(2)	N2	.H9	2.6000
O2	.C8	2.815(3)	C2	.C4	2.296(3)
O3	.S1_e	3.385(3)	C2	.C7_d	3.577(3)
O3	.C10_f	3.061(3)	N3	.H12	2.5400
O3	.C12	2.672(3)	N3	.H2	2.50(3)
O3	.C9_f	3.330(3)	C3	.N1_h	3.319(3)
O1	.H6A	2.4600	C3	.C6	3.053(3)
N1	.N3_g	3.175(3)	C3	.S1_g	3.6456(17)
N1	.C8_g	3.385(3)	C3	.S1	2.5639(18)
O1	.H11_c	2.4500	C4	.C2	2.296(3)
O1	.H6C_a	2.6500	C5	.C12_b	3.529(3)
N1	.C1	3.448(3)	C6	.C3	3.053(3)
N1	.C13_g	3.279(3)	C7	.C8_g	3.465(3)
N1	.C3_h	3.319(3)	C7	.N2	2.847(3)
N2	.O2	2.612(2)	C7	.C2_d	3.577(3)
N2	.C7	2.847(3)	C8	.C11	2.806(3)
O2	.H6B_d	2.7400	C8	.C7_a	3.465(3)
O2	.H2	1.94(3)	C8	.O2	2.815(3)

Table S8 - Contact Distances(Angstrom) (continued)
for: Polymorph_1 P 21/n R = 0.04

C8	.S1	3.288(2)	H2	.N3	2.50(3)
C8	.N1_a	3.385(3)	H2	.C2	2.55(3)
C9	.C1	3.030(3)	H2	.C7	2.55(3)
C9	.S1	3.132(2)	H2	.C9	3.07(3)
C9	.C12	2.740(3)	H2	.C13	2.47(3)
C9	.O3_c	3.330(3)	H3	.C5	2.8300
C10	.C13	2.722(3)	H3	.C6	2.8500
C10	.O3_c	3.061(3)	H3	.C7	2.7900
C11	.C8	2.806(3)	H3	.N1_h	2.5000
C11	.O1_f	3.213(3)	H6A	.O1	2.4600
C12	.C9	2.740(3)	H6B	.C3	3.0000
C12	.C5_e	3.529(3)	H6B	.C4	2.7600
C12	.O3	2.672(3)	H6B	.O2_d	2.7400
C13	.N1_a	3.279(3)	H6C	.O1_g	2.6500
C13	.C10	2.722(3)	H6C	.C3	3.0000
C1	.H9	2.7900	H6C	.C4	2.7400
C2	.H2	2.55(3)	H9	.S1	2.5300
C3	.H6B	3.0000	H9	.N2	2.6000
C3	.H6C	3.0000	H9	.C1	2.7900
C4	.H6B	2.7600	H9	.H10	2.2900
C4	.H6C	2.7400	H10	.H9	2.2900
C5	.H3	2.8300	H10	.H11	2.2900
C6	.H3	2.8500	H10	.O3_c	2.5200
C7	.H2	2.55(3)	H11	.H10	2.2900
C7	.H3	2.7900	H11	.H12	2.3000
C9	.H2	3.07(3)	H11	.O1_f	2.4500
C13	.H2	2.47(3)	H12	.O3	2.3700
H2	.O2	1.94(3)	H12	.N3	2.5400

Table S8 - Contact Distances(Angstrom) (continued)
for: Polymorph_1 P 21/n R = 0.04

H12	.H11	2.3000

Table S9 - Hydrogen Bonds (Angstrom, Deg)
for: Polymorph_1 P 21/n R = 0.04

N2	--	H2	..	O2	0.82(3)	1.94(3)	2.612(2)	139(3)	.
N2	--	H2	..	N3	0.82(3)	2.50(3)	2.884(3)	110(2)	.
C3	--	H3	..	N1	0.9300	2.5000	3.319(3)	147.00	3_466
C9	--	H9	..	S1	0.9300	2.5300	3.132(2)	123.00	.
C10	--	H10	..	O3	0.9300	2.5200	3.061(3)	117.00	2_646
C11	--	H11	..	O1	0.9300	2.4500	3.213(3)	139.00	2_656

Translation of Symmetry Code to Equiv.Pos

a =[1655.00] = [1_655] = 1+x,y,z
b =[2546.00] = [2_546] = 1/2-x,-1/2+y,3/2-z
c =[2646.00] = [2_646] = 3/2-x,-1/2+y,3/2-z
d =[3566.00] = [3_566] = -x,1-y,1-z
e =[2556.00] = [2_556] = 1/2-x,1/2+y,3/2-z
f =[2656.00] = [2_656] = 3/2-x,1/2+y,3/2-z
g =[1455.00] = [1_455] = -1+x,y,z
h =[3466.00] = [3_466] = -1-x,1-y,1-z