

## Reflex Summary Report for Rietveld Refinement of Etho\_dA(0)

Final $R_{wp}$ :	12.38%	Final $R_p$ :	8.61%
Final $R_{wp}$ (without background):	19.18%	Final CMACS:	2.37%

### Setup

$2\theta$ Range (degrees):	3.50-45.00	Step Size (degrees):	0.005
Experiment:	C1n.xcd		
Excluded Regions:	-		

### Radiation

Type:	X-ray	Source:	Copper
$\lambda$ (Å):	1.540562	Monochromator:	Single
dhkl:	1.000	Angle:	50.379
Anom. Dispersion:	No	Polarization:	0.900

### Lattice Parameters

Lattice Type:	Monoclinic	Space Group:	A 1 2/N 1
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Parameter	Value	Refined?
a	24.18398	No
b	4.73160	No
c	21.98316	No
$\alpha$	90.00000	No
$\beta$	114.62082	No
$\gamma$	90.00000	No

### Structure Parameters

Refined Motion Groups:	1	Refined Torsions:	3
Number of Refined DOF:	9		

### Fractional Coordinates

No.	Name	u	v	w	Refined?
1	C6	0.41556 ± 0.00009	0.99227 ± 0.00092	0.60212 ± 0.00013	Yes
2	C7	0.43382 ± 0.00009	0.86149 ± 0.00083	0.56103 ± 0.00013	Yes
3	C8	0.40017 ± 0.00010	0.72294 ± 0.00096	0.50314 ± 0.00015	Yes
4	C3	0.33578 ± 0.00010	0.72438 ± 0.00100	0.48621 ± 0.00014	Yes
5	C4	0.31468 ± 0.00009	0.86407 ± 0.00110	0.52967 ± 0.00013	Yes
6	C5	0.35402 ± 0.00009	1.00006 ± 0.00113	0.58819 ± 0.00014	Yes

7	N1	0.46252 ± 0.00010	1.10791 ± 0.00099	0.65555 ± 0.00014	Yes
8	C9	0.51489 ± 0.00010	1.05728 ± 0.00085	0.65191 ± 0.00012	Yes
9	S1	0.50884 ± 0.00009	0.85395 ± 0.00091	0.57870 ± 0.00013	Yes
10	S2	0.58813 ± 0.00011	1.17256 ± 0.00098	0.71233 ± 0.00012	Yes
11	O2	0.58474 ± 0.00016	1.45253 ± 0.00110	0.73317 ± 0.00030	Yes
12	O3	0.63447 ± 0.00010	1.08860 ± 0.00167	0.69270 ± 0.00020	Yes
13	N2	0.60150 ± 0.00021	0.98178 ± 0.00160	0.77981 ± 0.00017	Yes
14	O1	0.29800 ± 0.00012	0.58875 ± 0.00118	0.42823 ± 0.00016	Yes
15	C2	0.32280 ± 0.00019	0.36297 ± 0.00201	0.40416 ± 0.00029	Yes
16	C1	0.27268 ± 0.00023	0.20115 ± 0.00176	0.34810 ± 0.00032	Yes
17	H	0.41893 ± 0.00012	0.61803 ± 0.00116	0.47130 ± 0.00018	Yes
18	H	0.26580 ± 0.00009	0.86878 ± 0.00130	0.51809 ± 0.00014	Yes
19	H	0.33747 ± 0.00011	1.10766 ± 0.00142	0.62159 ± 0.00017	Yes
20	H	0.61031 ± 0.00021	1.13378 ± 0.00210	0.81411 ± 0.00012	Yes
21	H	0.64216 ± 0.00022	0.90069 ± 0.00132	0.78818 ± 0.00029	Yes
22	H	0.34810 ± 0.00071	0.21836 ± 0.00260	0.44589 ± 0.00036	Yes
23	H	0.35528 ± 0.00042	0.45030 ± 0.00366	0.38575 ± 0.00076	Yes
24	H	0.24745 ± 0.00050	0.34436 ± 0.00245	0.30616 ± 0.00029	Yes
25	H	0.24027 ± 0.00065	0.11238 ± 0.00260	0.36631 ± 0.00078	Yes
26	H	0.29131 ± 0.00033	0.02685 ± 0.00215	0.32922 ± 0.00036	Yes

#### Occupancies

No.	Name	Occupancy	Refined?
1	C6	1.00000	No
2	C7	1.00000	No
3	C8	1.00000	No
4	C3	1.00000	No
5	C4	1.00000	No
6	C5	1.00000	No
7	N1	1.00000	No
8	C9	1.00000	No
9	S1	1.00000	No
10	S2	1.00000	No
11	O2	1.00000	No
12	O3	1.00000	No
13	N2	1.00000	No
14	O1	1.00000	No
15	C2	1.00000	No
16	C1	1.00000	No
17	H	1.00000	No
18	H	1.00000	No
19	H	1.00000	No



24	H	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	No
25	H	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	No
26	H	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	No

## Pattern Parameters

Profile Function: Pseudo-Voigt

### FWHM

Parameter	Value	Refined?
U	0.36593 ± 0.01485	Yes
V	-0.05697 ± 0.00452	Yes
W	0.01360 ± 0.00033	Yes

### Profile

Parameter	Value	Refined?
NA	0.44816 ± 0.01401	Yes
NB	-0.00500 ± 0.00068	Yes

### Line Shift

Instrument Geometry: Bragg-Brentano

Parameter	Value	Refined?
Zero Point	-0.01786 ± 0.00051	Yes
Shift #1	0.00000	No
Shift #2	0.00000	No

### Asymmetry

Correction: Berar-Baldinazzi

2θ Limit: 90.000

Parameter	Value	Refined?
P1	-0.58690 ± 0.02111	Yes
P2	-0.26546 ± 0.00491	Yes
P3	0.97470 ± 0.04041	Yes
P4	0.48969 ± 0.01002	Yes

## Sample Parameters

### Preferred Orientation

Function: March-Dollase

Parameter	Value	Refined?
a*	-0.79224 ± 0.00249	Yes
b*	-0.42004 ± 0.00262	Yes

c*	$0.44263 \pm 0.00372$	Yes
R0	$1.95463 \pm 0.00782$	Yes