

Reflex Summary Report for Rietveld Refinement of Etho_dA(2)

Final R_{wp} :	9.24%	Final R_p :	6.76%
Final R_{wp} (without background):	14.44%	Final CMACS:	1.85%

Setup

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

Radiation

Type:	X-ray	Source:	Copper
λ (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	24.18400	No
b	4.73160	No
c	21.98320	No
α	90.00000	No
β	114.62080	No
γ	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	0.41695 ± 0.00008	0.98605 ± 0.00056	0.59313 ± 0.00009	Yes
2	C7	0.43747 ± 0.00007	0.83174 ± 0.00056	0.55103 ± 0.00008	Yes
3	C8	0.39761 ± 0.00008	0.68397 ± 0.00060	0.49465 ± 0.00009	Yes
4	C3	0.33575 ± 0.00008	0.69098 ± 0.00067	0.48113 ± 0.00011	Yes
5	C4	0.31489 ± 0.00007	0.84429 ± 0.00066	0.52292 ± 0.00012	Yes
6	C5	0.35440 ± 0.00008	0.99109 ± 0.00059	0.57807 ± 0.00011	Yes

7	N1	0.46236 ± 0.00009	1.11656 ± 0.00058	0.64684 ± 0.00008	Yes
8	C9	0.51556 ± 0.00008	1.06565 ± 0.00062	0.64716 ± 0.00007	Yes
9	S1	0.51572 ± 0.00007	0.86010 ± 0.00058	0.58173 ± 0.00008	Yes
10	S2	0.58579 ± 0.00009	1.17624 ± 0.00077	0.71201 ± 0.00008	Yes
11	O3	0.57919 ± 0.00015	1.47061 ± 0.00083	0.72451 ± 0.00022	Yes
12	O2	0.63107 ± 0.00008	1.08712 ± 0.00139	0.68967 ± 0.00017	Yes
13	N2	0.59453 ± 0.00018	1.01002 ± 0.00129	0.77902 ± 0.00011	Yes
14	O1	0.29166 ± 0.00009	0.55657 ± 0.00078	0.42925 ± 0.00013	Yes
15	C2	0.30890 ± 0.00013	0.37907 ± 0.00158	0.38632 ± 0.00028	Yes
16	C1	0.25296 ± 0.00020	0.21950 ± 0.00171	0.34057 ± 0.00030	Yes
17	H17	0.41408 ± 0.00010	0.56846 ± 0.00061	0.46275 ± 0.00010	Yes
18	H18	0.26643 ± 0.00008	0.84229 ± 0.00074	0.51080 ± 0.00014	Yes
19	H19	0.33769 ± 0.00009	1.10751 ± 0.00059	0.60977 ± 0.00012	Yes
20	H20	0.56946 ± 0.00020	1.09456 ± 0.00196	0.80348 ± 0.00008	Yes
21	H21	0.59513 ± 0.00024	0.79387 ± 0.00123	0.77458 ± 0.00023	Yes
22	H22	0.34493 ± 0.00041	0.23304 ± 0.00283	0.41792 ± 0.00046	Yes
23	H23	0.32696 ± 0.00062	0.51326 ± 0.00284	0.35790 ± 0.00058	Yes
24	H24	0.21768 ± 0.00033	0.36394 ± 0.00298	0.30756 ± 0.00039	Yes
25	H25	0.23398 ± 0.00072	0.09341 ± 0.00259	0.36923 ± 0.00062	Yes
26	H26	0.26545 ± 0.00023	0.07517 ± 0.00175	0.30935 ± 0.00032	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	O3	1.00000	No
12	O2	1.00000	No
13	N2	1.00000	No
14	O1	1.00000	No
15	C2	1.00000	No
16	C1	1.00000	No
17	H17	1.00000	No
18	H18	1.00000	No
19	H19	1.00000	No

24	H24	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	No
25	H25	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	No
26	H26	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	0.30856 ± 0.01044	Yes
V	-0.04058 ± 0.00325	Yes
W	0.01296 ± 0.00024	Yes

Profile

Parameter	Value	Refined?
NA	0.42681 ± 0.01017	Yes
NB	-0.00617 ± 0.00049	Yes

Line Shift

Instrument Geometry: Bragg-Brentano

Parameter	Value	Refined?
Zero Point	-0.01954 ± 0.00037	Yes
Shift #1	0.00000	No
Shift #2	0.00000	No

Asymmetry

Correction: Berar-Baldinazzi

2θ Limit: 90.000

Parameter	Value	Refined?
P1	-0.99237 ± 0.01544	Yes
P2	-0.35923 ± 0.00354	Yes
P3	1.79631 ± 0.02956	Yes
P4	0.67809 ± 0.00723	Yes

Sample Parameters

Preferred Orientation

Function: March-Dollase

Parameter	Value	Refined?
a*	-0.83073 ± 0.00113	Yes
b*	-0.38565 ± 0.00136	Yes

c*	0.40146 ± 0.00227	Yes
R0	1.96536 ± 0.00585	Yes