

Reflex Summary Report for Rietveld Refinement of CCl_2Br_2 (220K)

Final R_{wp} :	9.89%	Final R_{p} :	7.09%
Final R_{wp} (without background):	41.38%	Final CMACS:	1.25%

Setup

2 θ Range (degrees):	13.00-80.00	Step Size (degrees):	0.029
Experiment:	A1-220.xcd		
Excluded Regions:			

Radiation

Type:	X-ray	Source:	Copper
λ (Å):	1.540562	Monochromator:	Single
d hkl :	3.343	Angle:	13.320
Anom. Dispersion:	No	Polarization:	0.500

Lattice Parameters

Lattice Type: Monoclinic Space Group: C 1 2/C 1

Parameter	Value	Refined?
a	20.87229 ± 0.00105	Yes
b	11.74713 ± 0.00063	Yes
c	20.43362 ± 0.00077	Yes
α	90	No
β	111.18730 ± 0.00331	Yes
γ	90	No

Structure Parameters

Refined Motion Groups:	4	Refined Torsions:	0
Number of	24		

Refined DOF:

Fractional Coordinates

No.	Name	u	v	w	Refined?
1	C1	0.16628 ± 0.00101	0.80405 ± 0.00254	0.12640 ± 0.00109	Yes
2	CL11	0.18457 ± 0.00164	0.94894 ± 0.00253	0.14982 ± 0.00113	Yes
3	BR11	0.18630 ± 0.00173	0.96260 ± 0.00253	0.15203 ± 0.00114	Yes
4	CL12	0.08952 ± 0.00119	0.79442 ± 0.00281	0.05174 ± 0.00135	Yes
5	BR12	0.08229 ± 0.00122	0.79351 ± 0.00285	0.04471 ± 0.00139	Yes
6	CL13	0.15602 ± 0.00150	0.72927 ± 0.00302	0.19728 ± 0.00125	Yes
7	BR13	0.15505 ± 0.00159	0.72223 ± 0.00310	0.20396 ± 0.00128	Yes
8	CL14	0.23500 ± 0.00124	0.74356 ± 0.00330	0.10675 ± 0.00139	Yes
9	BR14	0.24148 ± 0.00128	0.73786 ± 0.00344	0.10489 ± 0.00145	Yes
10	C2	0.09336 ± 0.00110	0.97053 ± 0.00197	0.87479 ± 0.00098	Yes
11	CL21	0.02160 ± 0.00113	1.02227 ± 0.00237	0.89260 ± 0.00147	Yes
12	BR21	0.01484 ± 0.00114	1.02714 ± 0.00245	0.89429 ± 0.00154	Yes
13	CL22	0.08594 ± 0.00127	0.82117 ± 0.00198	0.86221 ± 0.00151	Yes
14	BR22	0.08524 ± 0.00131	0.80709 ± 0.00199	0.86102 ± 0.00161	Yes
15	CL23	0.16979 ± 0.00114	1.00221 ± 0.00271	0.94647 ± 0.00121	Yes
16	BR23	0.17699 ± 0.00115	1.00519 ± 0.00282	0.95324 ± 0.00124	Yes
17	CL24	0.09613 ± 0.00165	1.03647 ± 0.00278	0.79787 ± 0.00126	Yes
18	BR24	0.09640 ± 0.00173	1.04269 ± 0.00291	0.79061 ± 0.00130	Yes
19	C3	0.12804 ± 0.00106	0.69397 ± 0.00250	0.62567 ± 0.00088	Yes
20	CL31	0.13958 ± 0.00105	0.76030 ± 0.00350	0.70703 ± 0.00113	Yes
21	BR31	0.14066 ± 0.00105	0.76655 ± 0.00365	0.71469 ± 0.00117	Yes
22	CL32	0.05497 ± 0.00125	0.60415 ± 0.00289	0.60163 ± 0.00126	Yes
23	BR32	0.04808 ± 0.00129	0.59568 ± 0.00297	0.59936 ± 0.00132	Yes
24	CL33	0.20175 ± 0.00116	0.61192 ± 0.00322	0.63369 ± 0.00122	Yes
25	BR33	0.20869 ± 0.00118	0.60419 ± 0.00333	0.63445 ± 0.00129	Yes
26	CL34	0.11590 ± 0.00175	0.79950 ± 0.00280	0.56031 ± 0.00135	Yes
27	BR34	0.11475 ± 0.00185	0.80945 ± 0.00287	0.55415 ± 0.00142	Yes
28	C4	0.13061 ± 0.00121	0.54927 ± 0.00212	0.37575 ± 0.00092	Yes
29	CL41	0.20036 ± 0.00119	0.64491 ± 0.00251	0.39235 ± 0.00128	Yes
30	BR41	0.20693 ± 0.00120	0.65393 ± 0.00257	0.39392 ± 0.00136	Yes
31	CL42	0.05372 ± 0.00124	0.62733 ± 0.00244	0.35934 ± 0.00144	Yes
32	BR42	0.04648 ± 0.00126	0.63468 ± 0.00250	0.35780 ± 0.00154	Yes
33	CL43	0.14539 ± 0.00125	0.46024 ± 0.00327	0.44978 ± 0.00151	Yes
34	BR43	0.14678 ± 0.00126	0.45185 ± 0.00343	0.45676 ± 0.00158	Yes
35	CL44	0.12297 ± 0.00192	0.46460 ± 0.00302	0.30153 ± 0.00154	Yes

36	BR44	0.12225 ± 0.00201	0.45661 ± 0.00318	0.29454 ± 0.00162	Yes
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Occupancies

No.	Name	Occupancy	Refined?
1	C1	1.00000	No
2	CL11	0.50000	No
3	BR11	0.50000	No
4	CL12	0.50000	No
5	BR12	0.50000	No
6	CL13	0.50000	No
7	BR13	0.50000	No
8	CL14	0.50000	No
9	BR14	0.50000	No
10	C2	1.00000	No
11	CL21	0.50000	No
12	BR21	0.50000	No
13	CL22	0.50000	No
14	BR22	0.50000	No
15	CL23	0.50000	No
16	BR23	0.50000	No
17	CL24	0.50000	No
18	BR24	0.50000	No
19	C3	1.00000	No
20	CL31	0.50000	No
21	BR31	0.50000	No
22	CL32	0.50000	No
23	BR32	0.50000	No
24	CL33	0.50000	No
25	BR33	0.50000	No
26	CL34	0.50000	No
27	BR34	0.50000	No
28	C4	1.00000	No
29	CL41	0.50000	No
30	BR41	0.50000	No
31	CL42	0.50000	No
32	BR42	0.50000	No
33	CL43	0.50000	No
34	BR43	0.50000	No
35	CL44	0.50000	No

36	BR44	0.50000	No
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Pattern Parameters

Profile Function: Pseudo-Voigt

FWHM

Parameter	Value	Refined?
U	0.01710 ± 0.01118	Yes
V	-0.01164 ± 0.00728	Yes
W	0.00863 ± 0.00113	Yes

Profile

Parameter	Value	Refined?
NA	0.19192 ± 0.03882	Yes
NB	0.00000	No

Line Shift

Instrument
 Geometry: Debye-Scherrer

Parameter	Value	Refined?
Zero Point	0.00000	No
Shift #1	0.00000	No
Shift #2	0.00000	No

Sample Parameters

Preferred Orientation

Function: Rietveld-Toraya

Parameter	Value	Refined?
a [*]	0.31007 ± 0.00955	Yes
b [*]	-0.00000 ± 0.01443	Yes
c [*]	0.95071 ± 0.00312	Yes
G1	-6.69262 ± 0.49828	Yes
G2	0.19540 ± 0.00764	Yes

Global Isotropic Temperature Factors

Parameter	Value	Refined?
U	0.06762 ± 0.00294	Yes