

# Reflex Summary Report for Rietveld Refinement of $\text{CCl}_2\text{Br}_2$ (90K)

Final $R_{\text{wp}}$ :	9.16%	Final $R_{\text{p}}$ :	6.68%
Final $R_{\text{wp}}$ (without background):	36.73%	Final CMACS:	0.59%

## Setup

$2\theta$ Range (degrees):	13.00-80.00	Step Size (degrees):	0.029
Experiment:	A1-90.xcd		
Excluded Regions:	-		

## Radiation

Type:	X-ray	Source:	Copper
$\lambda$ (Å):	1.540562	Monochromator:	Single
dhkl:	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	$20.57424 \pm 0.00137$	Yes
b	$11.54684 \pm 0.00078$	Yes
c	$20.13418 \pm 0.00120$	Yes
$\alpha$	90	No
$\beta$	$111.68499 \pm 0.00369$	Yes
$\gamma$	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	C2	0.09357 ± 0.00101	0.96852 ± 0.00279	0.87329 ± 0.00098	Yes
2	CL21	0.02100 ± 0.00107	1.03210 ± 0.00296	0.88673 ± 0.00145	Yes
3	BR21	0.01417 ± 0.00107	1.03809 ± 0.00301	0.88800 ± 0.00152	Yes
4	CL22	0.07763 ± 0.00159	0.81885 ± 0.00267	0.85514 ± 0.00190	Yes
5	BR22	0.07612 ± 0.00166	0.80474 ± 0.00266	0.85342 ± 0.00202	Yes
6	CL23	0.16958 ± 0.00135	0.98663 ± 0.00413	0.95126 ± 0.00122	Yes
7	BR23	0.17675 ± 0.00139	0.98833 ± 0.00429	0.95862 ± 0.00127	Yes
8	CL24	0.10608 ± 0.00156	1.03655 ± 0.00298	0.80002 ± 0.00134	Yes
9	BR24	0.10726 ± 0.00168	1.04296 ± 0.00306	0.79311 ± 0.00141	Yes
10	C3	0.12471 ± 0.00123	0.68998 ± 0.00213	0.61973 ± 0.00116	Yes
11	CL31	0.13579 ± 0.00123	0.77623 ± 0.00219	0.69593 ± 0.00116	Yes
12	BR31	0.13682 ± 0.00123	0.78437 ± 0.00219	0.70311 ± 0.00116	Yes
13	CL32	0.05158 ± 0.00150	0.59757 ± 0.00266	0.60281 ± 0.00156	Yes
14	BR32	0.04469 ± 0.00155	0.58885 ± 0.00276	0.60121 ± 0.00162	Yes
15	CL33	0.20079 ± 0.00135	0.60531 ± 0.00285	0.63541 ± 0.00120	Yes
16	BR33	0.20795 ± 0.00138	0.59733 ± 0.00296	0.63689 ± 0.00121	Yes
17	CL34	0.11070 ± 0.00191	0.78081 ± 0.00210	0.54476 ± 0.00116	Yes
18	BR34	0.10938 ± 0.00201	0.78937 ± 0.00210	0.53769 ± 0.00116	Yes
19	C4	0.11911 ± 0.00110	0.43484 ± 0.00211	0.87780 ± 0.00110	Yes
20	CL41	0.19490 ± 0.00116	0.34847 ± 0.00204	0.89577 ± 0.00137	Yes
21	BR41	0.20204 ± 0.00116	0.34033 ± 0.00205	0.89746 ± 0.00142	Yes
22	CL42	0.04506 ± 0.00124	0.34405 ± 0.00248	0.85933 ± 0.00129	Yes
23	BR42	0.03809 ± 0.00126	0.33549 ± 0.00252	0.85759 ± 0.00136	Yes
24	CL43	0.12886 ± 0.00127	0.52230 ± 0.00306	0.95319 ± 0.00143	Yes
25	BR43	0.12978 ± 0.00130	0.53054 ± 0.00318	0.96030 ± 0.00147	Yes
26	CL44	0.10763 ± 0.00148	0.52454 ± 0.00215	0.80289 ± 0.00152	Yes
27	BR44	0.10655 ± 0.00155	0.53299 ± 0.00221	0.79583 ± 0.00157	Yes
28	C1	0.84160 ± 0.00107	0.21439 ± 0.00263	0.87941 ± 0.00087	Yes
29	CL11	0.82844 ± 0.00136	0.06526 ± 0.00265	0.85788 ± 0.00089	Yes
30	BR11	0.82720 ± 0.00143	0.05120 ± 0.00265	0.85585 ± 0.00089	Yes
31	CL12	0.91798 ± 0.00170	0.23209 ± 0.00270	0.95705 ± 0.00122	Yes
32	BR12	0.92518 ± 0.00177	0.23375 ± 0.00272	0.96437 ± 0.00128	Yes
33	CL13	0.85149 ± 0.00124	0.29027 ± 0.00271	0.80723 ± 0.00107	Yes
34	BR13	0.85242 ± 0.00131	0.29742 ± 0.00274	0.80043 ± 0.00110	Yes
35	CL14	0.76846 ± 0.00174	0.26996 ± 0.00339	0.89548 ± 0.00172	Yes

36	BR14	$0.76157 \pm 0.00182$	$0.27520 \pm 0.00351$	$0.89700 \pm 0.00184$	Yes
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## Occupancies

No.	Name	Occupancy	Refined?
1	C2	1.00000	No
2	CL21	0.50000	No
3	BR21	0.50000	No
4	CL22	0.50000	No
5	BR22	0.50000	No
6	CL23	0.50000	No
7	BR23	0.50000	No
8	CL24	0.50000	No
9	BR24	0.50000	No
10	C3	1.00000	No
11	CL31	0.50000	No
12	BR31	0.50000	No
13	CL32	0.50000	No
14	BR32	0.50000	No
15	CL33	0.50000	No
16	BR33	0.50000	No
17	CL34	0.50000	No
18	BR34	0.50000	No
19	C4	1.00000	No
20	CL41	0.50000	No
21	BR41	0.50000	No
22	CL42	0.50000	No
23	BR42	0.50000	No
24	CL43	0.50000	No
25	BR43	0.50000	No
26	CL44	0.50000	No
27	BR44	0.50000	No
28	C1	1.00000	No
29	CL11	0.50000	No
30	BR11	0.50000	No
31	CL12	0.50000	No
32	BR12	0.50000	No
33	CL13	0.50000	No
34	BR13	0.50000	No
35	CL14	0.50000	No

36	BR14	0.50000	No
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## Pattern Parameters

Profile Function: Pseudo-Voigt

### FWHM

Parameter	Value	Refined?
U	$0.01375 \pm 0.01272$	Yes
V	$0.01521 \pm 0.00843$	Yes
W	$0.00376 \pm 0.00128$	Yes

### Profile

Parameter	Value	Refined?
NA	$0.38537 \pm 0.03433$	Yes
NB	0.00000	No

### Line Shift

Instrument  
Geometry: Debye-Scherrer

Parameter	Value	Refined?
Zero Point	$-0.00433 \pm 0.00148$	Yes
Shift #1	0.00000	No
Shift #2	0.00000	No

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## Sample Parameters

### Preferred Orientation

Function: Rietveld-Toraya

Parameter	Value	Refined?
a <sup>*</sup>	$0.15313 \pm 0.01460$	Yes
b <sup>*</sup>	$-0.00000 \pm 0.01108$	Yes
c <sup>*</sup>	$0.98821 \pm 0.00226$	Yes
G1	$-8.60954 \pm 0.52184$	Yes
G2	$0.23395 \pm 0.00706$	Yes

### Global Isotropic Temperature Factors

<b>Parameter</b>	<b>Value</b>	<b>Refined?</b>
U	$0.01582 \pm 0.00156$	Yes