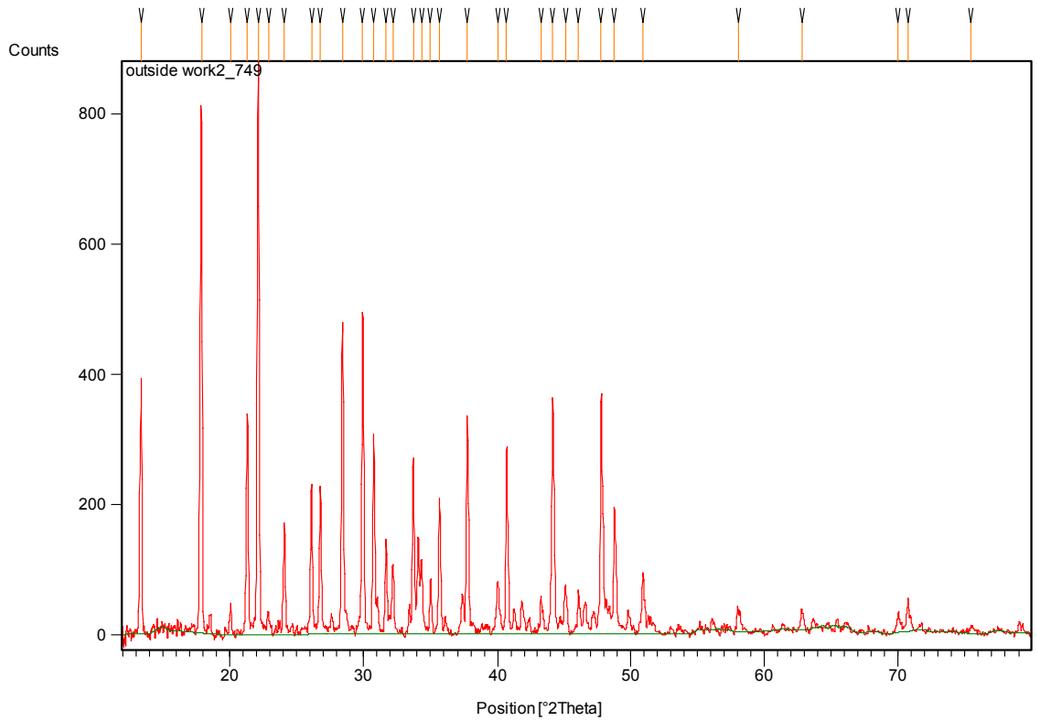
Powder Diffraction Data for Pure KHP

This is the simple example template containing only headers for each report item and the bookmarks. The invisible bookmarks are indicated by text between brackets.
Modify it according to your own needs and standards.

Measurement Conditions: (Bookmark 1)

Dataset Name	outside work2_749
File name	C:\X'Pert Data\outside work2_749.xrdml
Sample Identification	Pure Potassium Hydrogen phalate (KHP)
Measurement Date / Time	8/31/2007 3:09:10 PM
Operator	Central Electrochem
Raw Data Origin	XRD measurement (*.XRDML)
Scan Axis	Gonio
Start Position [°2Th.]	11.9594
End Position [°2Th.]	79.9934
Step Size [°2Th.]	0.0170
Scan Step Time [s]	20.6753
Scan Type	Continuous
PSD Mode	Scanning
PSD Length [°2Th.]	2.12
Offset [°2Th.]	0.0000
Divergence Slit Type	Fixed
Divergence Slit Size [°]	0.9570
Specimen Length [mm]	10.00
Measurement Temperature [°C]	25.00
Anode Material	Cu
K-Alpha1 [Å]	1.54060
K-Alpha2 [Å]	1.54443
K-Beta [Å]	1.39225
K-A2 / K-A1 Ratio	0.50000
Generator Settings	30 mA, 40 kV
Diffractometer Type	0000000083004288
Diffractometer Number	0
Goniometer Radius [mm]	240.00
Dist. Focus-Diverg. Slit [mm]	91.00
Incident Beam Monochromator	No
Spinning	No

Main Graphics, Analyze View: (Bookmark 2)



Peak List: (Bookmark 3)

Pos. [°2Th.]	Height [cts]	FWHM [°2Th.]	d-spacing [Å]	Rel. Int. [%]
13.4062	365.43	0.1004	6.60476	43.85
17.8968	767.79	0.2007	4.95637	92.13
20.0695	49.18	0.1673	4.42443	5.90
21.3268	338.06	0.1840	4.16635	40.56
22.1474	833.41	0.1840	4.01381	100.00
22.9139	25.93	0.2676	3.88124	3.11
24.0903	170.24	0.2007	3.69430	20.43
26.1031	229.47	0.1338	3.41383	27.53
26.7704	226.15	0.1338	3.33023	27.14
28.4325	479.10	0.1840	3.13922	57.49
29.9285	494.76	0.1673	2.98562	59.37
30.7497	308.89	0.1338	2.90774	37.06
31.6757	143.93	0.1338	2.82481	17.27
32.1902	102.70	0.1338	2.78083	12.32
33.7008	270.01	0.1338	2.65956	32.40
34.3570	102.78	0.3346	2.61025	12.33
34.9981	83.03	0.2007	2.56390	9.96
35.6459	205.91	0.1673	2.51877	24.71
37.7321	327.24	0.1338	2.38417	39.27
40.0155	79.76	0.2676	2.25323	9.57
40.6730	281.39	0.1004	2.21831	33.76
43.3535	44.17	0.4015	2.08717	5.30
44.1922	360.26	0.2007	2.04949	43.23
45.1438	75.50	0.3011	2.00847	9.06
46.1071	65.61	0.2007	1.96873	7.87
47.8149	359.65	0.1004	1.90232	43.15
48.8084	191.73	0.1673	1.86590	23.01
50.9691	77.76	0.2676	1.79176	9.33
58.0516	32.19	0.3346	1.58889	3.86
62.8410	29.26	0.2676	1.47883	3.51
69.9879	23.06	0.4015	1.34429	2.77
70.7279	42.30	0.2676	1.33203	5.08
75.4649	7.50	0.9792	1.25871	0.90

Pattern List: (Bookmark 4)

Document History: (Bookmark 5)

Insert Measurement:
- File name = "outside work2_749.xrdml"
- Modification time = "8/31/2007 3:24:11 PM"
- Modification editor = "Central Electrochem"

Default properties:
- Measurement step axis = "None"
- Internal wavelengths used from anode material: Copper (Cu)
- Original K-Alpha1 wavelength = "1.54060"
- Used K-Alpha1 wavelength = "1.54060"
- Original K-Alpha2 wavelength = "1.54443"
- Used K-Alpha2 wavelength = "1.54443"
- Original K-Beta wavelength = "1.39225"
- Used K-Beta wavelength = "1.39225"
- Incident beam monochromator = "No"
- Dist. focus to div. slit = "91.00000"
- Irradiated length = "10.00000"
- Spinner used = "No"
- Step axis value = "0.00000"
- Offset = "0.00000"
- Sample length = "10.00000"
- Modification time = "8/31/2007 3:24:11 PM"
- Modification editor = "Central Electrochem"

Interpolate Step Size:
- Step Size = "Derived"
- Modification time = "11/1/2004"
- Modification editor = "PANalytical"

Smooth:
- Type of smoothing = "Polynomial"
- Polynomial type = "Cubic"
- Convolution range = "9"
- Modification time = "8/23/2007 2:06:24 PM"
- Modification editor = "Central Electrochem"

Subtract Background:
- Correction method = "Automatic"
- Bending factor = "0"
- Use smoothed input data = "Yes"
- Granularity = "25"
- Add to net scan = "Nothing"
- Modification time = "8/2/2007 2:50:47 PM"
- Modification editor = "Central Electrochem"

Search Peaks:
- Minimum significance = "6.00"
- Minimum tip width = "0.01"
- Maximum tip width = "1.00"
- Peak base width = "1.50"
- Method = "Minimum 2nd derivative"
- Modification time = "8/31/2007 3:15:33 PM"
- Modification editor = "Central Electrochem"

Search Peaks:
- Minimum significance = "8.00"
- Minimum tip width = "0.01"
- Maximum tip width = "1.00"
- Peak base width = "1.50"
- Method = "Minimum 2nd derivative"
- Modification time = "8/31/2007 3:24:36 PM"
- Modification editor = "Central Electrochem"

More items… (Bookmark 6)

More items… (Bookmark 7)

More items… (Bookmark 8)

More items… (Bookmark 9)

More items… (Bookmark 10)

More items… (Bookmark 11)

More items… (Bookmark 12)

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More items… (Bookmark 14)

More items… (Bookmark 15)

Powder Diffraction Data for KHP Doped with 20 mol% Mg

This is the simple example template containing only headers for each report item and the bookmarks. The invisible bookmarks are indicated by text between brackets.
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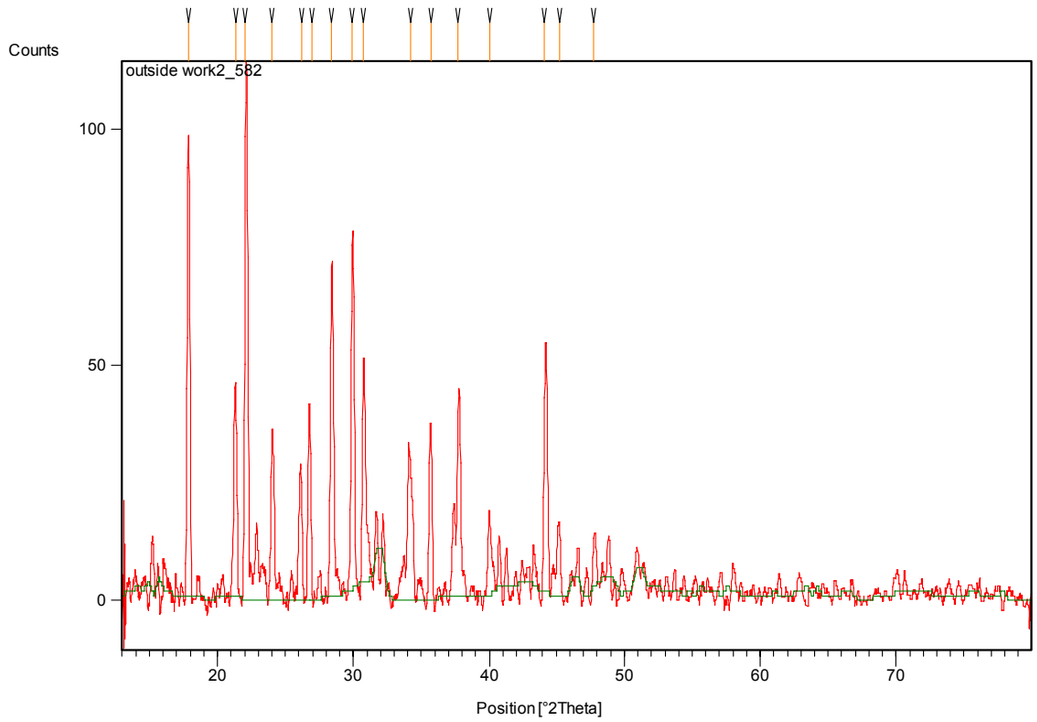
Measurement Conditions: (Bookmark 1)

Dataset Name	outside work2_582
File name	C:\X'Pert Data\outside work2_582.xrdml
Sample Identification	**KHP/20mol% Mg doping**
Measurement Date / Time	7/16/2007 2:54:40 PM
Operator	Central Electrochem
Raw Data Origin	XRD measurement (*.XRDML)
Scan Axis	Gonio
Start Position [°2Th.]	12.9924
End Position [°2Th.]	79.9894
Step Size [°2Th.]	0.0170
Scan Step Time [s]	10.9840
Scan Type	Continuous
PSD Mode	Scanning
PSD Length [°2Th.]	2.12
Offset [°2Th.]	0.0000
Divergence Slit Type	Fixed
Divergence Slit Size [°]	0.9570
Specimen Length [mm]	10.00
Measurement Temperature [°C]	25.00
Anode Material	Cu
K-Alpha1 [Å]	1.54060
K-Alpha2 [Å]	1.54443
K-Beta [Å]	1.39225
K-A2 / K-A1 Ratio	0.50000
Generator Settings	30 mA, 40 kV
Diffractometer Type	0000000083004288
Diffractometer Number	0
Goniometer Radius [mm]	240.00
Dist. Focus-Diverg. Slit [mm]	91.00
Incident Beam Monochromator	No
Spinning	No

Main Graphics, Analyze View: (Bookmark 2)



Peak List: (Bookmark 3)

Pos. [°2Th.]	Height [cts]	FWHM [°2Th.]	d-spacing [Å]	Rel. Int. [%]
17.8650	97.28	0.2175	4.96512	100.00
21.3358	45.16	0.2676	4.16462	46.42
22.0691	97.20	0.2844	4.02787	99.92
24.0104	34.31	0.3011	3.70641	35.27
26.1928	22.54	0.2844	3.40234	23.17
26.9490	5.97	0.2844	3.30857	6.14
28.4145	70.33	0.2342	3.14117	72.30
29.9111	70.70	0.2844	2.98732	72.68
30.7518	46.12	0.2007	2.90754	47.41
34.1900	29.33	0.4015	2.62262	30.15
35.7595	30.78	0.3178	2.51103	31.64
37.7099	38.19	0.6691	2.38552	39.26
40.0165	15.24	0.4015	2.25318	15.66
44.1258	38.16	0.2844	2.05241	39.23
45.2247	15.15	0.2676	2.00507	15.58
47.7813	11.15	0.3264	1.90201	11.46

Pattern List: (Bookmark 4)

Document History: (Bookmark 5)

Insert Measurement:
- File name = "outside work2_582.xrdml"
- Modification time = "7/16/2007 4:37:16 PM"
- Modification editor = "Central Electrochem"

Default properties:
- Measurement step axis = "None"
- Internal wavelengths used from anode material: Copper (Cu)
- Original K-Alpha1 wavelength = "1.54060"
- Used K-Alpha1 wavelength = "1.54060"
- Original K-Alpha2 wavelength = "1.54443"
- Used K-Alpha2 wavelength = "1.54443"
- Original K-Beta wavelength = "1.39225"
- Used K-Beta wavelength = "1.39225"

- Incident beam monochromator = "No"
- Dist. focus to div. slit = "91.00000"
- Irradiated length = "10.00000"
- Spinner used = "No"
- Receiving slit size = "0.10000"
- Step axis value = "0.00000"
- Offset = "0.00000"
- Sample length = "10.00000"
- Modification time = "7/16/2007 4:37:16 PM"
- Modification editor = "Central Electrochem"

Interpolate Step Size:
- Step Size = "Derived"
- Modification time = "11/1/2004"
- Modification editor = "PANalytical"

Smooth:
- Type of smoothing = "Polynomial"
- Polynomial type = "Cubic"
- Convolution range = "25"
- Modification time = "4/5/2007 4:32:43 PM"
- Modification editor = "Central Electrochem"

Subtract Background:
- Correction method = "Automatic"
- Bending factor = "3"
- Use smoothed input data = "Yes"
- Granularity = "13"
- Add to net scan = "Nothing"
- Modification time = "5/4/2007 4:17:06 PM"
- Modification editor = "Central Electrochem"

Search Peaks:
- Minimum significance = "8.00"
- Minimum tip width = "0.01"
- Maximum tip width = "1.00"
- Peak base width = "1.50"
- Method = "Minimum 2nd derivative"
- Modification time = "7/16/2007 4:24:26 PM"
- Modification editor = "Central Electrochem"

More items… (Bookmark 6)

More items… (Bookmark 7)

More items… (Bookmark 8)

More items… (Bookmark 9)

More items… (Bookmark 10)

More items… (Bookmark 11)

More items… (Bookmark 12)

More items… (Bookmark 13)

More items… (Bookmark 14)

More items… (Bookmark 15)

Powder Diffraction Data for KHP Doped with Mg(I)

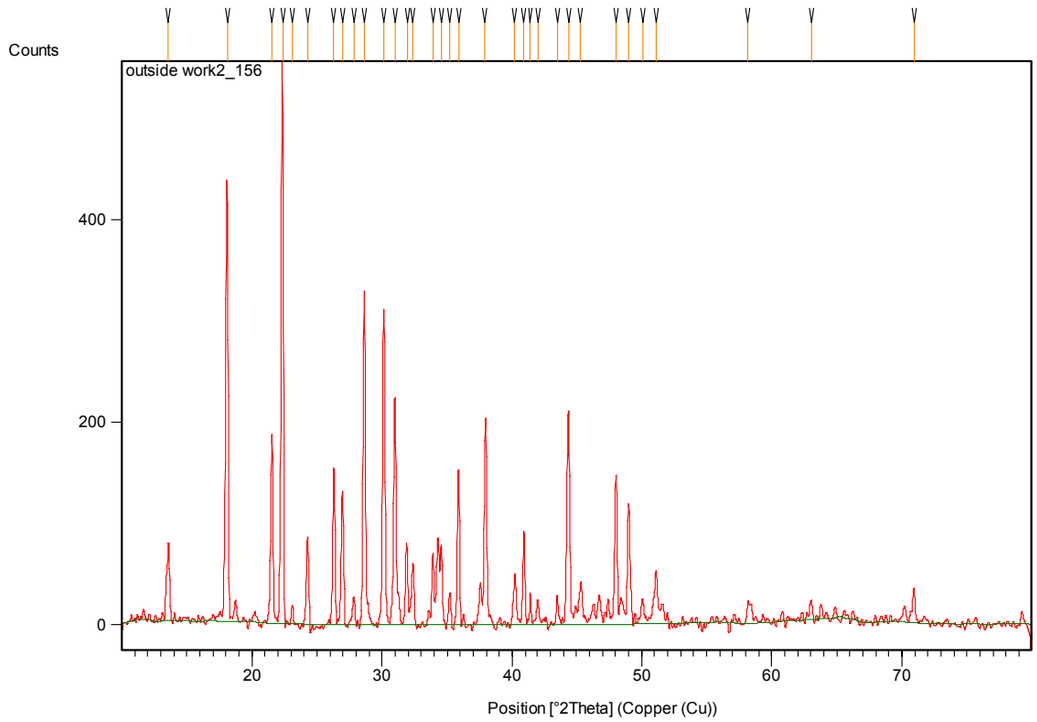
This is the simple example template containing only headers for each report item and the bookmarks. The invisible bookmarks are indicated by text between brackets.
Modify it according to your own needs and standards.

Measurement Conditions: (Bookmark 1)

Dataset Name	outside work2_156
File name	C:\X'Pert Data\outside work2_156.xrdml
Sample Identification	KMG1(KHP doped with Mg(I))
Measurement Date / Time	8/13/2008 11:27:14 AM
Operator	Central Electrochem
Raw Data Origin	XRD measurement (*.XRDML)
Scan Axis	Gonio
Start Position [°2Th.]	10.0214
End Position [°2Th.]	79.9764
Step Size [°2Th.]	0.0170
Scan Step Time [s]	21.9677
Scan Type	Continuous
PSD Mode	Scanning
PSD Length [°2Th.]	2.12
Offset [°2Th.]	0.0000
Divergence Slit Type	Fixed
Divergence Slit Size [°]	0.9570
Specimen Length [mm]	10.00
Measurement Temperature [°C]	25.00
Anode Material	Cu
K-Alpha1 [Å]	1.54060
Generator Settings	30 mA, 40 kV
Diffractometer Type	0000000083004288
Diffractometer Number	0
Goniometer Radius [mm]	240.00
Dist. Focus-Diverg. Slit [mm]	91.00
Incident Beam Monochromator	No
Spinning	No

Main Graphics, Analyze View: (Bookmark 2)

Peak List: (Bookmark 3)



Pattern List: (Bookmark 4)

Pos. [°2Th.]	Height [cts]	FWHM [°2Th.]	d-spacing [Å]	Rel. Int. [%]
13.5236	64.99	0.3264	6.54228	17.22
18.1085	377.31	0.2040	4.89485	100.00
21.5524	178.30	0.1632	4.11983	47.26
22.3919	371.60	0.1836	3.96725	98.49
23.0972	18.85	0.2448	3.84767	5.00
24.2453	85.26	0.2040	3.66801	22.60
26.2499	140.61	0.1632	3.39226	37.27
26.9590	132.60	0.2856	3.30462	35.14
27.7965	26.58	0.2448	3.20692	7.05
28.6399	320.56	0.2040	3.11438	84.96
30.1183	311.53	0.1428	2.96478	82.57
30.9714	223.52	0.2040	2.88504	59.24
31.9036	73.50	0.2040	2.80284	19.48
32.3712	57.49	0.2448	2.76341	15.24
33.8837	69.46	0.1632	2.64343	18.41
34.5501	72.44	0.1632	2.59396	19.20
35.2119	30.43	0.2040	2.54670	8.07
35.8894	136.42	0.1632	2.50017	36.16
37.8943	195.38	0.1836	2.37237	51.78
40.1586	45.33	0.2448	2.24367	12.01
40.8887	91.31	0.1836	2.20528	24.20
41.4099	30.30	0.2448	2.17872	8.03
42.0279	23.29	0.2448	2.14810	6.17
43.5310	28.26	0.1224	2.07735	7.49
44.4095	200.24	0.2856	2.03827	53.07
45.3154	40.22	0.2448	1.99961	10.66
48.0591	139.17	0.2448	1.89166	36.88
48.9912	117.15	0.1632	1.85783	31.05
50.0784	24.13	0.4896	1.82001	6.39
51.1072	52.11	0.3264	1.78576	13.81
58.1734	20.36	0.4080	1.58454	5.40
63.0215	18.55	0.2448	1.47381	4.92
70.9091	33.76	0.3264	1.32797	8.95

Document History: (Bookmark 5)

More items… (Bookmark 6)

More items… (Bookmark 7)

More items… (Bookmark 8)

More items… (Bookmark 9)

More items… (Bookmark 10)

More items… (Bookmark 11)

More items… (Bookmark 12)

More items… (Bookmark 13)

More items… (Bookmark 14)

More items… (Bookmark 15)

Powder Diffraction Data for KHP Doped with Hg

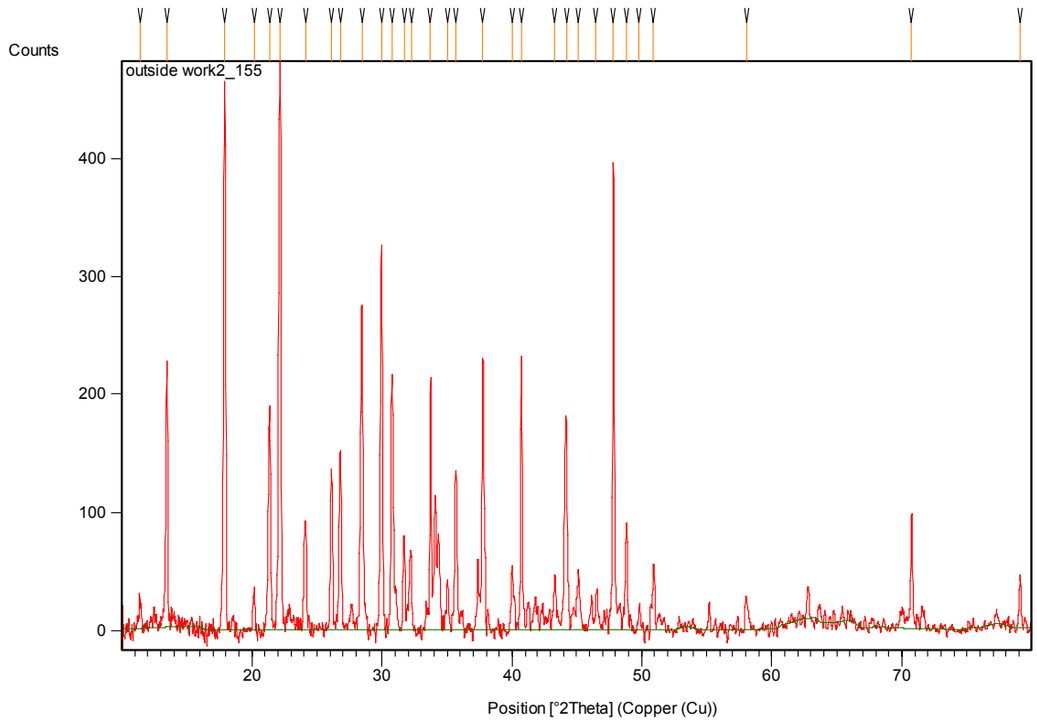
This is the simple example template containing only headers for each report item and the bookmarks. The invisible bookmarks are indicated by text between brackets.
Modify it according to your own needs and standards.

Measurement Conditions: (Bookmark 1)

Dataset Name	outside work2_155
File name	C:\X'Pert Data\outside work2_155.xrdml
Sample Identification	KHG(KHP doped with Hg)
Measurement Date / Time	8/13/2008 11:10:38 AM
Operator	Central Electrochem
Raw Data Origin	XRD measurement (*.XRDML)
Scan Axis	Gonio
Start Position [°2Th.]	10.0214
End Position [°2Th.]	79.9764
Step Size [°2Th.]	0.0170
Scan Step Time [s]	21.9677
Scan Type	Continuous
PSD Mode	Scanning
PSD Length [°2Th.]	2.12
Offset [°2Th.]	0.0000
Divergence Slit Type	Fixed
Divergence Slit Size [°]	0.9570
Specimen Length [mm]	10.00
Measurement Temperature [°C]	25.00
Anode Material	Cu
K-Alpha1 [Å]	1.54060
Generator Settings	30 mA, 40 kV
Diffractometer Type	0000000083004288
Diffractometer Number	0
Goniometer Radius [mm]	240.00
Dist. Focus-Diverg. Slit [mm]	91.00
Incident Beam Monochromator	No
Spinning	No

Main Graphics, Analyze View: (Bookmark 2)

Peak List: (Bookmark 3)



Pattern List: (Bookmark 4)

Pos. [°2Th.]	Height [cts]	FWHM [°2Th.]	d-spacing [Å]	Rel. Int. [%]
11.4124	23.31	0.3264	7.74734	5.03
13.4719	218.32	0.1836	6.56726	47.08
17.8868	463.68	0.2652	4.95501	100.00
20.1463	33.21	0.2448	4.40408	7.16
21.3804	179.46	0.2040	4.15259	38.70
22.1843	441.13	0.2856	4.00389	95.14
24.1358	87.16	0.3264	3.68439	18.80
26.1046	135.58	0.2448	3.41081	29.24
26.8063	149.79	0.2856	3.32310	32.30
28.4353	274.33	0.3264	3.13632	59.16
29.9269	321.32	0.2448	2.98331	69.30
30.7246	206.05	0.2652	2.90765	44.44
31.7160	68.51	0.2652	2.81898	14.78
32.2380	54.54	0.2652	2.77452	11.76
33.7146	211.57	0.1224	2.65630	45.63
35.0173	40.05	0.2448	2.56041	8.64
35.6479	137.04	0.2448	2.51655	29.55
37.7402	230.38	0.1836	2.38170	49.69
39.9920	49.34	0.3264	2.25263	10.64
40.7044	233.09	0.1428	2.21484	50.27
43.2973	35.48	0.3264	2.08802	7.65
44.2203	178.00	0.2856	2.04655	38.39
45.1167	39.80	0.4896	2.00795	8.58
46.4276	16.56	0.9792	1.95426	3.57
47.8460	395.20	0.1224	1.89959	85.23
48.8585	87.54	0.2244	1.86256	18.88
49.8090	17.37	0.3264	1.82922	3.75
50.9187	54.89	0.2448	1.79193	11.84
58.0364	27.04	0.3264	1.58796	5.83
70.7383	96.37	0.1632	1.33076	20.78
79.0582	38.57	0.2448	1.21027	8.32

Document History: (Bookmark 5)

More items… (Bookmark 6)

More items… (Bookmark 7)

More items… (Bookmark 8)

More items… (Bookmark 9)

More items… (Bookmark 10)

More items… (Bookmark 11)

More items… (Bookmark 12)

More items… (Bookmark 13)

More items… (Bookmark 14)

More items… (Bookmark 15)

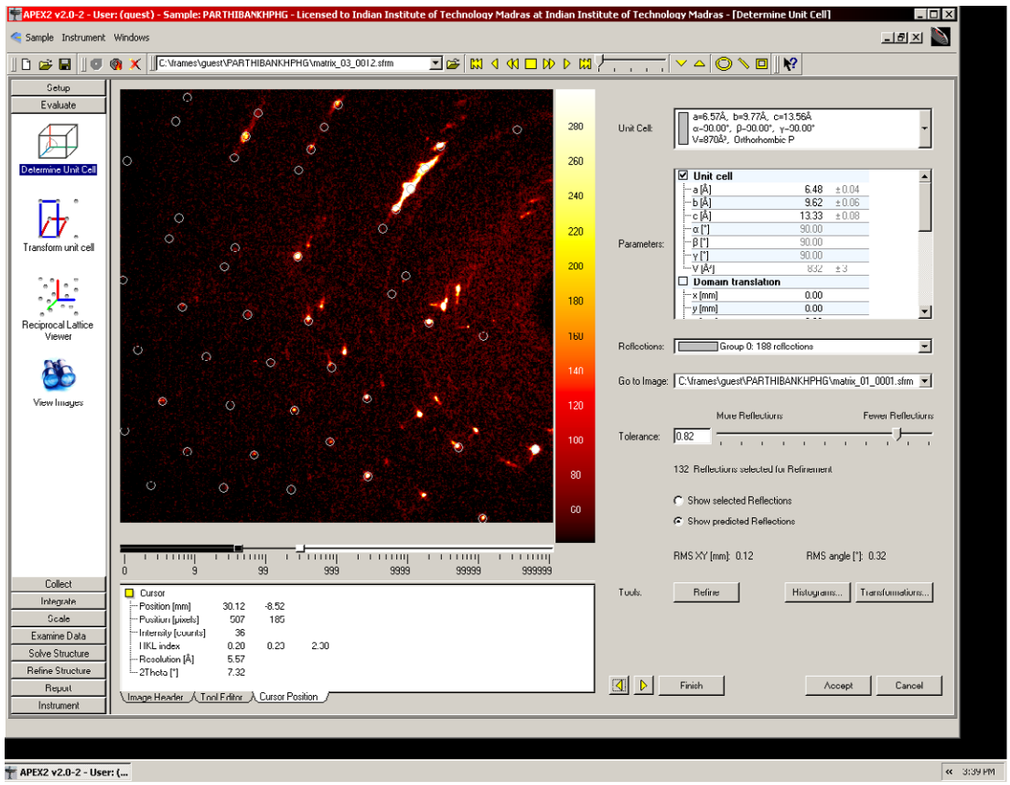


Fig. S1 Cell parameter values for a KHP crystal doped with Hg(I)

Cell parameter values for heavy Mg-doping – Single crystal XRD instrument generated values

REIND

Nr	S	H	K	L	Dev-Ang	dTh	dPh	dCh
0.0075177								
1	H	-2.000	-2.981	-1.053	0.5621	0.032	-0.540	0.157
0.0044308								
2	H	-1.991	-3.008	-1.003	0.1974	0.014	-0.029	-0.195
0.0015678								
3	H	-1.999	-3.000	0.996	0.0413	0.005	-0.040	-0.010
0.0003380								
4	H	-1.994	-2.025	-4.012	0.3205	-0.053	0.002	-0.320
0.0029049								
5	H	-1.996	-2.019	-2.995	0.2699	-0.016	0.111	-0.246
0.0020835								
6	H	-1.998	-2.015	-1.997	0.2170	-0.024	0.076	-0.203
0.0016132								
7	H	-2.000	-2.002	0.007	0.0856	-0.005	0.080	-0.033
0.0005674								
8	H	-0.004	-3.008	-3.965	0.3395	0.057	0.376	-0.129
0.0028480								
9	H	-0.010	-2.954	-5.007	0.4916	0.127	-0.287	0.423
0.0049719								
10	H	-0.995	-4.011	-1.959	0.4123	0.012	0.409	-0.187
0.0033911								
12	H	-0.997	-4.013	0.039	0.3901	-0.051	0.422	-0.103
0.0032162								
13	H	-0.997	-3.992	-1.024	0.2436	0.028	-0.272	-0.016
0.0020076								
14	H	-1.002	-4.007	0.981	0.1933	-0.026	-0.215	-0.014
0.0016176								
15	H	-3.012	-0.985	-0.997	0.2377	-0.068	0.031	0.236
0.0024572								
16	H	-3.004	-0.997	1.007	0.0742	-0.030	0.066	0.047
0.0008880								
17	H	2.994	1.996	2.009	0.1039	0.037	-0.108	0.013
0.0012221								

```
18 H    2.994    1.996  -1.986    0.0744      0.063  -0.078  -0.005

0.0014752
19 H    3.021   -2.011   2.000    0.1109     -0.159   0.218  -0.032

0.0034557
20 H    1.988    4.002   3.985    0.1609      0.070   0.033   0.157

0.0021981
21 H   -1.982    3.996   4.032    0.3546      0.024   0.262  -0.330

0.0037478
23 H    2.019    3.987  -4.011    0.3008     -0.050   0.002  -0.301

0.0033017
Reciprocal axis matrix                  Direct axis matrix
  -0.015393  -0.012177   0.074238        -0.582994  -4.722684
4.396364
  -0.113051  -0.069443  -0.011561        -1.239489  -6.374848  -
7.114616
   0.103978  -0.076212  -0.002575        13.146032  -2.024868  -
0.255459□□□
Niggli-values                           Sigma direct axis matrix
    41.9716    92.7928   176.9835         0.012740   0.005552
0.010741
    -1.5686     0.7757    -0.4494         0.020564   0.008962
0.017338
                                         0.030150   0.013139
0.025421□□□
Cell parameters                         Sigma cell parameters
     6.4786     9.6329    13.3035           0.0084     0.0144
  0.0299
    90.7014    89.4844    90.4126           0.1511     0.1409
  0.1123
  -0.012241   0.009000  -0.007202         0.002637   0.002459
0.001960
 Volume=      830.1192                               2.4834
Index-Status: HHHHHHHHHH/HHHHHHHHHH/H//
CD0> LO
□From to: 1 25
□ 1H  -2.  -3.  -1. * 20.09 S   0.53   18.62    3.69 **S   1 1.
66
4827.4
 2H  -2.  -3.  -1. * 20.11 S  -0.39   18.75    4.15 **S   1 1.2
2
9718.2
 3H  -2.  -3.   1. * 20.10 S -19.35   19.02    3.05 **S   1 1.2
7
9805.2
 4H  -2.  -2.  -4. * 21.71 S  32.67   23.78   -6.65 **S   1 1.2
8
16188.1
```

```
 5H  -2.  -2.  -3. * 19.64 S  24.83   22.52   -7.90 **S   1 0.8
2
1609.8
 6H  -2.  -2.  -2. * 18.08 S  16.19   21.21   -9.13 **S   1 0.9
4
4336.0
 7H  -2.  -2.   0. * 16.72 S  -5.10   20.31  -11.13 **S   1 1.1
4
25760.9
 8H   0.  -3.  -4. * 19.55 S  30.34    5.27   44.06 **S   1 1.1
6
6516.3
 9H   0.  -3.  -5. * 22.10 S  39.57    9.27   38.20 **S   1 1.1
9
10565.9
10H  -1.  -4.  -2. * 21.21 S  -0.52   10.30   34.40 **S   1 1.2
2
20810.8
11N   0.  -3.  -5. * 22.10 S  40.62    9.91   36.43 **S   1 1.4
0
4533.5
12H  -1.  -4.   0. * 20.05 S -21.10    8.21   35.48 **S   1 1.1
5
13125.1
13H  -1.  -4.  -1. * 20.30 S  -9.74    8.68   35.26 **S   1 1.5
2
4139.0
14H  -1.  -4.   1. * 20.30 S -31.04    9.02   34.38 **S   1 1.4
0
4012.8
15H  -3.  -1.  -1. * 21.80 S  14.78   34.44  -38.48 **S   1 1.4
1
2588.4
16H  -3.  -1.   1. * 21.81 S  -5.69   34.67  -39.09 **S   1 1.1
1
4458.8
17H   3.   2.   2. * 24.07 S-178.35   17.03   22.14 **S   1 1.3
8
13309.0
18H   3.   2.  -2. * 24.08 S 146.65   16.47   23.65 **S   1 1.7
1
18555.6
19H   3.  -2.   2. * 24.07 S 179.91   -5.46   82.70 **S   1 1.3
4
2301.3
20H   2.   4.   4. * 27.52 S-154.07   31.90  -13.63 **S   1 1.5
3
4941.5
21H  -2.   4.   4. * 27.55 S -80.23   56.50  -81.77 **S   1 1.5
0
4690.0
23H   2.   4.  -4. * 27.52 S 143.92   30.89  -10.47 **S   1 1.6
```