Data Sheet 3.1. Peak search and intensity data of XRD of Pyrolusite ore containing with 85% MnO_2 used in their dye manufacture by M/s Atul Ltd.

K-Alpha1 wavelength (Å):	1.54056
K-Alpha2 wavelength (Å):	1.54439
K-Alpha2/K-Alpha1 intensity ratio :	0.50000
K-Alpha wavelength (Å):	1.54056
K-Beta wavelength (Å):	1.39222

Peak search parameter set:	**As Measured Intensities**
Set created	2/21/03 13:11
Peak positions defined by:	Minimum of 2nd derivative
Minimum peak tip width (°2Theta):	0.00
Minimum peak tip width (°2Theta):	1.50
Peak base width (°2Theta):	3.00
Minimum significance:	0.60

d-spacing (Å)	Relative Intensity (%)	Angle (°2Theta)	Peak Height (counts/s)	Background (counts/s)	Tip Width (°2Theta)	Significance
6.96604	1.11	12.69709	3.16	4.50	1.00000	0.86
3.99670	9.88	22.22419	28.13	10.07	0.50000	1.30
3.34364	12.25	26.63794	34.89	9.09	0.10000	1.89
3.11657	100.00	28.61860	284.85	8.92	0.20000	3.94
2.70066	21.53	33.14395	61.33	8.66	0.15000	2.91
2.58579	7.03	34.66184	20.04	8.61	0.40000	1.52
2.51633	10.83	35.65025	30.85	8.57	0.25000	1.66
2.43293	29.31	36.91560	83.49	8.52	0.20000	0.61
2.40679	46.85	37.33122	133.45	8.51	0.20000	1.12
2.34293	14.69	38.38796	41.83	8.47	0.40000	0.89
2.20357	11.66	40.92089	33.22	8.38	0.30000	1.91
2.13693	17.68	42.25708	50.36	8.33	0.30000	2.12
2.10929	18.31	42.83792	52.15	8.31	0.20000	0.94
2.05333	3.39	44.06547	9.65	8.26	0.60000	1.41
1.97349	4.22	45.94799	12.01	8.22	0.30000	1.52
1.89202	2.88	48.04809	8.20	8.20	1.00000	1.16
1.83965	7.78	49.50636	22.16	8.19	0.30000	0.68
1.69363	7.64	54.10556	21.75	8.32	0.30000	0.61
1.62576	51.47	56.56198	146.62	8.46	0.30000	2.22
1.55693	19.10	59.30553	54.42	8.61	0.25000	1.39
1.48612	8.88	62.43861	25.31	8.79	0.40000	0.76
1.43670	11.11	64.84343	31.66	8.93	0.20000	0.85
1.35503	12.68	69.28561	36.13	9.18	0.30000	0.61
1.30479	23.30	72.36330	66.37	9.36	0.90000	5.81
1.24822	2.55	76.20973	7.28	9.58	0.80000	0.69

Data Sheet 3.2 (a). Peak search and intensity data of XRD of $MnCO_3$ sample fused at 450 °C for 4 h containing 58.45% MnO_2

Original scan: Mn11	Date: 12/29/06 13:13
Description of scan: 29-12-06	
Used wavelength:	K-Alpha1
K-Alpha1 wavelength (Å):	1.54056
K-Alpha2 wavelength (Å):	1.54439
K-Alpha2/K-Alpha1 intensity ratio :	0.50000
K-Alpha wavelength (Å):	1.54056
K-Beta wavelength (Å):	1.39222
Peak search parameter set:	**As Measured Intensities**
Set created:	2/21/03 13:11
Peak positions defined by:	Minimum of 2nd derivative
Minimum peak tip width (°2Theta):	0.00
Minimum peak tip width (°2Theta):	1.00
Peak base width (°2Theta):	2.00
Minimum significance:	0.60

d-spacing (Å)	Relative Intensity (%)	Angle (°2Theta)	Peak Height (counts/s)	Background (counts/s)	Tip Width (°2Theta)	Significance
2.44466	100.00	36.73214	34.96	56.89	0.80000	1.11

Data Sheet 3.2 (b). Peak search and intensity data of XRD of $MnCO_3$ sample fused at 450 °C for 6 h containing 53.89% MnO_2.

K-Alpha1 wavelength (Å):	1.54056
K-Alpha2 wavelength (Å):	1.54439
K-Alpha2/K-Alpha1 intensity ratio :	0.50000
K-Alpha wavelength (Å):	1.54056
K-Beta wavelength (Å):	1.39222

Peak search parameter set:	**As Measured Intensities**
Set created:	2/21/03 13:11
Peak positions defined by:	Minimum of 2nd derivative
Minimum peak tip width (°2Theta):	0.00
Minimum peak tip width (°2Theta):	1.00
Peak base width (°2Theta):	2.00
Minimum significance:	0.60

d-spacing (Å)	Relative Intensity (%)	Angle (°2Theta)	Peak Height (counts/s)	Background (counts/s)	Tip Width (°2Theta)	Significance
2.40833	100.00	37.30651	39.24	53.78	0.60000	1.22
1.80860	15.92	50.41510	6.25	39.80	0.60000	0.61
1.65540	40.68	55.46100	15.97	41.16	0.25000	0.69

Data Sheet 3.2 (c). Peak search and intensity data of XRD of $MnCO_3$ sample fused at 450 °C for 2.5 h containing 84% MnO_2 after HCl treatment

Used wavelength:	K-Alpha1
K-Alpha1 wavelength (Å):	1.54056
K-Alpha2 wavelength (Å):	1.54439
K-Alpha2/K-Alpha1 intensity ratio :	0.50000
K-Alpha wavelength (Å):	1.54056
K-Beta wavelength (Å):	1.39222
Peak search parameter set:	**As Measured Intensities**
Set created:	2/21/03 13:11
Peak positions defined by:	Minimum of 2nd derivative
Minimum peak tip width (°2Theta):	0.00
Minimum peak tip width (°2Theta):	1.00
Peak base width (°2Theta):	2.00
Minimum significance:	0.60

d-spacing (Å)	Relative Intensity (%)	Angle (°2Theta)	Peak Height (counts/s)	Background (counts/s)	Tip Width (°2Theta)	Significance
2.41753	100.00	37.15934	98.94	45.91	0.15000	0.74
2.13546	32.55	42.28745	32.20	34.41	1.00000	2.21
1.64931	30.31	55.68356	29.99	51.59	0.60000	0.77
1.02436	7.60	97.52183	7.52	20.71	0.25000	0.94

Data Sheet 3.3 (a). Peak search and intensity data of XRD of $MnCO_3$ fused sample along with 1 g Na_2CO_3 at 500 °C for 3 h sample containing 73.66% MnO_2.

Used wavelength:	K-Alpha1
K-Alpha1 wavelength (Å):	1.54056
K-Alpha2 wavelength (Å):	1.54439
K-Alpha2/K-Alpha1 intensity ratio :	0.50000
K-Alpha wavelength (Å):	1.54056
K-Beta wavelength (Å):	1.39222
Peak search parameter set:	**As Measured Intensities**
Set created:	2/21/03 13:11
Peak positions defined by:	Minimum of 2nd derivative
Minimum peak tip width (°2Theta):	0.00
Minimum peak tip width (°2Theta):	1.00
Peak base width (°2Theta):	2.00
Minimum significance:	0.60

d-spacing (Å)	Relative Intensity (%)	Angle (°2Theta)	Peak Height (counts/s)	Background (counts/s)	Tip Width (°2Theta)	Significance
9.40913	23.65	9.39157	7.72	10.33	0.80000	2.18
6.75714	27.34	13.09132	8.93	14.06	1.00000	1.00
2.44545	100.00	36.71987	32.66	37.72	0.60000	1.41
1.42192	46.16	65.60155	15.07	35.01	0.80000	0.95
1.35794	40.83	69.11629	13.34	28.95	0.15000	0.70

Data Sheet 3.3 (b). Peak search and intensity data of XRD of $MnCO_3$ fused sample along with 1.93 g Na_2CO_3 at 500 °C for 3 h containing 73.88% MnO_2

Used wavelength:	K-Alpha1
K-Alpha1 wavelength (Å):	1.54056
K-Alpha2 wavelength (Å):	1.54439
K-Alpha2/K-Alpha1 intensity ratio :	0.50000
K-Alpha wavelength (Å):	1.54056
K-Beta wavelength (Å):	1.39222
Peak search parameter set:	**As Measured Intensities**
Set created:	2/21/03 13:11
Peak positions defined by:	Minimum of 2nd derivative
Minimum peak tip width (°2Theta):	0.00
Minimum peak tip width (°2Theta):	1.00
Peak base width (°2Theta):	2.00
Minimum significance:	0.60

d-spacing (Å)	Relative Intensity (%)	Angle (°2Theta)	Peak Height (counts/s)	Background (counts/s)	Tip Width (°2Theta)	Significance
6.73976	45.68	13.12523	20.22	12.65	0.50000	0.77
4.63368	3.10	19.13796	1.37	14.67	0.50000	0.63
2.41365	100.00	37.22115	44.26	32.77	0.70000	2.22
1.40728	61.44	66.37138	27.19	33.23	1.00000	2.04

Data Sheet 3.3 (c). Peak search and intensity data of XRD of $MnCO_3$ fused sample along with 3.9 g Na_2CO_3 at 500 °C for 3 h containing 75.40% MnO_2

Used wavelength:	K-Alpha1
K-Alpha1 wavelength (Å):	1.54056
K-Alpha2 wavelength (Å):	1.54439
K-Alpha2/K-Alpha1 intensity ratio :	0.50000
K-Alpha wavelength (Å):	1.54056
K-Beta wavelength (Å):	1.39222
Peak search parameter set:	**As Measured Intensities**
Set created:	2/21/03 13:11
Peak positions defined by:	Minimum of 2nd derivative
Minimum peak tip width (°2Theta):	0.00
Minimum peak tip width (°2Theta):	1.00
Peak base width (°2Theta):	2.00
Minimum significance:	0.60

d-spacing (Å)	Relative Intensity (%)	Angle (°2Theta)	Peak Height (counts/s)	Background (counts/s)	Tip Width (°2Theta)	Significance
9.22711	9.92	9.57726	4.73	9.41	0.80000	0.67
6.88918	31.09	12.83934	14.84	12.22	1.00000	1.78
3.83818	7.92	23.15449	3.78	15.25	0.50000	0.61
3.51119	16.95	25.34506	8.09	18.37	0.30000	0.72
2.43360	100.00	36.90511	47.74	37.09	0.60000	2.62
1.52635	31.52	60.61690	15.04	25.83	0.25000	0.76

Data Sheet 3.4(a). Peak search and intensity data of XRD of $MnCO_3$ sample fused along with 5 g Na_2CO_3 at 450 °C for 2.5 h

Used wavelength:	K-Alpha1
K-Alpha1 wavelength (Å):	1.54056
K-Alpha2 wavelength (Å):	1.54439
K-Alpha2/K-Alpha1 intensity ratio :	0.50000
K-Alpha wavelength (Å):	1.54056
K-Beta wavelength (Å):	1.39222
Peak search parameter set:	**As Measured Intensities**
Set created:	2/21/03 13:11
Peak positions defined by:	Minimum of 2nd derivative
Minimum peak tip width (°2Theta):	0.00
Minimum peak tip width (°2Theta):	1.00
Peak base width (°2Theta):	2.00
Minimum significance:	0.60

d-spacing (Å)	Relative Intensity (%)	Angle (°2Theta)	Peak Height (counts/s)	Background (counts/s)	Tip Width (°2Theta)	Significance
9.42911	26.93	9.37163	16.33	15.56	0.70000	1.34
6.89287	31.19	12.83245	18.91	20.47	0.60000	1.21
2.43941	100.00	36.81399	60.64	56.04	0.40000	0.78
1.21400	10.87	78.76561	6.59	27.26	0.80000	0.62

Data Sheet 3.4(b). Peak search and intensity data of XRD of $MnCO_3$ sample fused along with 10 g Na_2CO_3 at 450 °C for 2.5 h.

Used wavelength:	K-Alpha1
K-Alpha1 wavelength (Å):	1.54056
K-Alpha2 wavelength (Å):	1.54439
K-Alpha2/K-Alpha1 intensity ratio :	0.50000
K-Alpha wavelength (Å):	1.54056
K-Beta wavelength (Å):	1.39222
Peak search parameter set:	**As Measured Intensities**
Set created:	2/21/03 13:11
Peak positions defined by:	Minimum of 2nd derivative
Minimum peak tip width (°2Theta):	0.00
Minimum peak tip width (°2Theta):	1.00
Peak base width (°2Theta):	2.00
Minimum significance:	0.60

d-spacing (Å)	Relative Intensity (%)	Angle (°2Theta)	Peak Height (counts/s)	Background (counts/s)	Tip Width (°2Theta)	Significance
9.59281	14.12	9.21135	11.14	14.65	0.60000	1.01
3.14749	24.55	28.33153	19.38	24.09	0.10000	0.64
3.01706	16.19	29.58367	12.78	24.57	0.30000	0.76
2.42570	100.00	37.02959	78.92	48.79	0.90000	5.99
1.40658	61.95	66.40846	48.89	44.37	0.40000	0.67

Data Sheet 3.4(c). Peak search and intensity data of XRD of $MnCO_3$ sample fused along with 15 g Na_2CO_3 at 450 °C for 2.5 h

Used wavelength:	K-Alpha1
K-Alpha1 wavelength (Å):	1.54056
K-Alpha2 wavelength (Å):	1.54439
K-Alpha2/K-Alpha1 intensity ratio :	0.50000
K-Alpha wavelength (Å):	1.54056
K-Beta wavelength (Å):	1.39222
Peak search parameter set:	**As Measured Intensities**
Set created:	2/21/03 13:11
Peak positions defined by:	Minimum of 2nd derivative
Minimum peak tip width (°2Theta):	0.00
Minimum peak tip width (°2Theta):	1.00
Peak base width (°2Theta):	2.00
Minimum significance:	0.60

d-spacing (Å)	Relative Intensity (%)	Angle (°2Theta)	Peak Height (counts/s)	Background (counts/s)	Tip Width (°2Theta)	Significance
9.88344	5.59	8.93993	4.70	17.13	0.80000	0.63
7.01508	35.61	12.60797	29.95	29.89	0.50000	0.88
4.85110	12.68	18.27272	10.66	20.81	0.40000	0.61
2.44481	100.00	36.72974	84.10	43.14	0.15000	0.82
1.41542	72.59	65.94074	61.05	43.73	0.40000	0.75

Data Sheet 3.4(d). Peak search and intensity data of XRD of $MnCO_3$ sample fused along with 20 g Na_2CO_3 at 450 °C for 2.5 h.

Used wavelength:	K-Alpha1
K-Alpha1 wavelength (Å):	1.54056
K-Alpha2 wavelength (Å):	1.54439
K-Alpha2/K-Alpha1 intensity ratio :	0.50000
K-Alpha wavelength (Å):	1.54056
K-Beta wavelength (Å):	1.39222
Peak search parameter set:	**As Measured Intensities**
Set created:	2/21/03 13:11
Peak positions defined by:	Minimum of 2nd derivative
Minimum peak tip width (°2Theta):	0.00
Minimum peak tip width (°2Theta):	1.00
Peak base width (°2Theta):	2.00
Minimum significance:	0.60

d-spacing (Å)	Relative Intensity (%)	Angle (°2Theta)	Peak Height (counts/s)	Background (counts/s)	Tip Width (°2Theta)	Significance
13.34994	0.53	6.61551	14.69	11.96	0.20000	0.68
11.44755	0.23	7.71644	6.45	11.07	0.25000	0.97
9.48335	0.14	9.31791	4.00	12.24	1.00000	0.63
6.92680	2.94	12.76933	81.23	18.44	0.40000	1.86
3.42726	0.47	25.97645	12.96	23.84	0.80000	1.53
3.25191	2.38	27.40378	65.66	25.47	0.15000	0.74
2.81504	100.00	31.76076	2760.88	24.62	0.15000	10.05
2.42579	2.15	37.02820	59.41	41.30	0.50000	1.95
2.18551	0.74	41.27432	20.53	38.59	0.60000	1.06
1.99248	18.55	45.48536	512.18	26.77	0.20000	5.92
1.69706	0.71	53.98707	19.59	33.22	0.30000	1.19
1.62829	6.59	56.46647	182.02	35.22	0.25000	2.68
1.40955	19.75	66.25060	545.33	44.44	0.15000	1.94
1.26091	11.16	75.30828	308.04	23.71	0.15000	2.17
1.25713	4.00	75.57388	110.39	23.87	0.10000	2.69
1.17797	0.15	81.67295	4.01	21.03	0.50000	0.65
1.15111	4.66	84.00541	128.56	21.56	0.15000	1.09
1.14792	2.15	84.29166	59.29	21.74	0.15000	0.67
1.08547	0.67	90.40957	18.51	20.66	0.15000	0.62

Data Sheet 3.5(a) Peak search and intensity data of XRD of $MnCO_3$ sample fused along with 2 g $CaCO_3$ at 450 °C for 2.5 h

Used wavelength:	K-Alpha1
K-Alpha1 wavelength (Å):	1.54056
K-Alpha2 wavelength (Å):	1.54439
K-Alpha2/K-Alpha1 intensity ratio :	0.50000
K-Alpha wavelength (Å):	1.54056
K-Beta wavelength (Å):	1.39222
Peak search parameter set:	**As Measured Intensities**
Set created:	2/21/03 13:11
Peak positions defined by:	Minimum of 2nd derivative
Minimum peak tip width (°2Theta):	0.00
Minimum peak tip width (°2Theta):	1.00
Peak base width (°2Theta):	2.00
Minimum significance:	0.60

d-spacing (Å)	Relative Intensity (%)	Angle (°2Theta)	Peak Height (counts/s)	Background (counts/s)	Tip Width (°2Theta)	Significance
2.42973	100.00	36.96592	70.50	54.74	0.20000	0.63
2.13755	44.65	42.24408	31.48	33.09	0.80000	1.45
1.39758	27.80	66.89202	19.60	45.91	0.80000	0.61

Data Sheet 3.5(b). Peak search and intensity data of XRD of $MnCO_3$ sample fused along with 2 g $MgCO_3$ at 450 °C for 2.5 h.

Used wavelength:	K-Alpha1
K-Alpha1 wavelength (Å):	1.54056
K-Alpha2 wavelength (Å):	1.54439
K-Alpha2/K-Alpha1 intensity ratio :	0.50000
K-Alpha wavelength (Å):	1.54056
K-Beta wavelength (Å):	1.39222
Peak search parameter set:	**As Measured Intensities**
Set created:	2/21/03 13:11
Peak positions defined by:	Minimum of 2nd derivative
Minimum peak tip width (°2Theta):	0.00
Minimum peak tip width (°2Theta):	1.00
Peak base width (°2Theta):	2.00
Minimum significance:	0.60

d-spacing (Å)	Relative Intensity (%)	Angle (°2Theta)	Peak Height (counts/s)	Background (counts/s)	Tip Width (°2Theta)	Significance
2.74025	100.00	32.65157	633.41	31.30	0.15000	4.87
2.42934	10.87	36.97216	68.83	47.10	0.60000	2.44
2.14261	4.78	42.13961	30.29	37.10	1.00000	1.62

Data Sheet 3.6(a). Peak search and intensity data of XRD of $MnCO_3$ fused sample at 450 °C along with 0.1 g NaOH for 2 h having 59.75% MnO_2.

Used wavelength:	K-Alpha1
K-Alpha1 wavelength (Å):	1.54056
K-Alpha2 wavelength (Å):	1.54439
K-Alpha2/K-Alpha1 intensity ratio :	0.50000
K-Alpha wavelength (Å):	1.54056
K-Beta wavelength (Å):	1.39222
Peak search parameter set:	**As Measured Intensities**
Set created:	2/21/03 13:11
Peak positions defined by:	Minimum of 2nd derivative
Minimum peak tip width (°2Theta):	0.00
Minimum peak tip width (°2Theta):	1.00
Peak base width (°2Theta):	2.00
Minimum significance:	0.60

d-spacing (Å)	Relative Intensity (%)	Angle (°2Theta)	Peak Height (counts/s)	Background (counts/s)	Tip Width (°2Theta)	Significance
4.84048	36.10	18.31317	12.04	21.94	0.50000	0.87
2.81404	96.89	31.77239	32.32	38.69	0.15000	1.09
2.47213	100.00	36.30961	33.36	53.05	1.00000	1.44
1.62961	22.64	56.41633	7.55	40.71	0.60000	0.63
1.49148	59.94	62.18916	20.00	43.81	0.15000	0.69

Data Sheet 3.6(b). Peak search and intensity data of XRD of $MnCO_3$ fused sample at 450 °C along with 1.0 g NaOH for 3 h having 69.10% MnO_2.

Used wavelength:	K-Alpha1
K-Alpha1 wavelength (Å):	1.54056
K-Alpha2 wavelength (Å):	1.54439
K-Alpha2/K-Alpha1 intensity ratio :	0.50000
K-Alpha wavelength (Å):	1.54056
K-Beta wavelength (Å):	1.39222
Peak search parameter set:	**As Measured Intensities**
Set created:	2/21/03 13:11
Peak positions defined by:	Minimum of 2nd derivative
Minimum peak tip width (°2Theta):	0.00
Minimum peak tip width (°2Theta):	1.00
Peak base width (°2Theta):	2.00
Minimum significance:	0.60

d-spacing (Å)	Relative Intensity (%)	Angle (°2Theta)	Peak Height (counts/s)	Background (counts/s)	Tip Width (°2Theta)	Significance
7.03054	67.03	12.58014	25.42	16.75	0.80000	1.59
3.53247	19.97	25.18986	7.57	20.75	0.60000	0.96
2.81878	73.10	31.71760	27.73	20.11	0.30000	1.79
2.44326	100.00	36.75391	37.93	36.50	0.50000	0.77
1.99624	60.13	45.39503	22.81	24.74	0.15000	1.00

Data Sheet 3.6(c). Peak search and intensity data of XRD of $MnCO_3$ fused sample at 450 °C along with 1.0 g NaOH for 4 h having 61.27% MnO_2

Used wavelength:	K-Alpha1
K-Alpha1 wavelength (Å):	1.54056
K-Alpha2 wavelength (Å):	1.54439
K-Alpha2/K-Alpha1 intensity ratio :	0.50000
K-Alpha wavelength (Å):	1.54056
K-Beta wavelength (Å):	1.39222
Peak search parameter set:	**As Measured Intensities**
Set created:	2/21/03 13:11
Peak positions defined by:	Minimum of 2nd derivative
Minimum peak tip width (°2Theta):	0.00
Minimum peak tip width (°2Theta):	1.00
Peak base width (°2Theta):	2.00
Minimum significance:	0.60

d-spacing (Å)	Relative Intensity (%)	Angle (°2Theta)	Peak Height (counts/s)	Background (counts/s)	Tip Width (°2Theta)	Significance
2.42416	100.00	37.05405	48.50	60.81	0.30000	0.97
2.13797	16.53	42.23545	8.02	46.61	1.00000	0.83

Data Sheet 3.7. Peak search and intensity data of XRD of 55.5% MnO_2 obtained by the chemical oxidation of Mn(II) in ME using Cl_2 gas.

Used wavelength:	K-Alpha1
K-Alpha1 wavelength (Å):	1.54056
K-Alpha2 wavelength (Å):	1.54439
K-Alpha2/K-Alpha1 intensity ratio :	0.50000
K-Alpha wavelength (Å):	1.54056
K-Beta wavelength (Å):	1.39222
Peak search parameter set:	**As Measured Intensities**
Set created:	2/21/03 13:11
Peak positions defined by:	Minimum of 2nd derivative
Minimum peak tip width (°2Theta):	0.00
Minimum peak tip width (°2Theta):	1.00
Peak base width (°2Theta):	2.00
Minimum significance:	0.60

d-spacing (Å)	Relative Intensity (%)	Angle (°2Theta)	Peak Height (counts/s)	Background (counts/s)	Tip Width (°2Theta)	Significance
2.40220	100.00	37.40518	37.79	41.19	0.30000	0.64
1.40862	87.17	66.30026	32.94	39.53	1.00000	1.61

Data Sheet 3.8. Peak search and intensity data of XRD of 88% MnO_2 obtained by the chemical oxidation of Mn(II) in ME using $NaBrO_3$.

Used wavelength	K-Alpha1
K-Alpha1 wavelength (Å):	1.54056
K-Alpha2 wavelength (Å):	1.54439
K-Alpha2/K-Alpha1 intensity ratio :	0.50000
K-Alpha wavelength (Å):	1.54056
K-Beta wavelength (Å):	1.39222
Peak search parameter set:	**As Measured Intensities**
Set created:	2/21/03 13:11
Peak positions defined by:	Minimum of 2nd derivative
Minimum peak tip width (°2Theta):	0.00
Minimum peak tip width (°2Theta):	1.50
Peak base width (°2Theta):	3.00
Minimum significance:	0.60

d-spacing (Å)	Relative Intensity (%)	Angle (°2Theta)	Peak Height (counts/s)	Background (counts/s)	Tip Width (°2Theta)	Significance
6.99923	18.58	12.63663	13.84	10.40	0.60000	2.15
4.93176	32.62	17.97135	24.30	19.43	0.30000	1.97
4.73213	30.09	18.73619	22.42	22.51	0.30000	1.20
3.19321	60.67	27.91760	45.19	21.72	0.50000	2.26
2.59929	24.50	34.47617	18.25	19.34	0.30000	1.09
2.43885	99.96	36.82268	74.46	22.11	0.15000	0.70
2.39537	100.00	37.51579	74.49	22.93	0.50000	1.50
2.14929	43.60	42.00241	32.48	28.24	1.20000	1.92
1.82842	19.58	49.83097	14.59	20.34	0.60000	2.13
1.67889	35.71	54.61978	26.60	19.92	0.60000	0.63
1.64304	63.16	55.91476	47.05	20.49	0.80000	1.03
1.53715	25.32	60.14686	18.86	22.36	0.60000	1.36
1.42540	33.44	65.42124	24.91	21.88	0.40000	0.71
1.40007	48.47	66.75772	36.11	21.88	0.80000	1.01
1.35184	32.26	69.47251	24.03	21.88	0.30000	0.77
1.29590	14.21	72.93937	10.59	21.88	0.60000	0.68

Data Sheet 3.9. Peak search and intensity data of XRD of 80% MnO_2 obtained by the chemical oxidation of Mn(II) in ME using $KMnO_4$.

Used wavelength:	K-Alpha1
K-Alpha1 wavelength (Å):	1.54056
K-Alpha2 wavelength (Å):	1.54439
K-Alpha2/K-Alpha1 intensity ratio :	0.50000
K-Alpha wavelength (Å):	1.54056
K-Beta wavelength (Å):	1.39222
Peak search parameter set:	**As Measured Intensities**
Set created:	2/21/03 13:11
Peak positions defined by:	Minimum of 2nd derivative
Minimum peak tip width (°2Theta):	0.00
Minimum peak tip width (°2Theta):	1.00
Peak base width (°2Theta):	2.00
Minimum significance:	0.60

d-spacing (Å)	Relative Intensity (%)	Angle (°2Theta)	Peak Height (counts/s)	Background (counts/s)	Tip Width (°2Theta)	Significance
6.94160	28.37	12.74198	62.13	18.53	0.30000	0.75
4.93139	27.75	17.97274	60.77	22.99	0.60000	3.04
3.47719	3.00	25.59710	6.56	21.24	0.60000	0.67
3.09051	45.87	28.86514	100.44	33.19	0.25000	0.90
2.38507	100.00	37.68398	218.97	38.74	0.30000	2.58
2.14702	49.12	42.04903	107.57	27.47	0.20000	0.72
1.92619	5.02	47.14373	11.00	22.67	0.60000	1.00
1.82572	47.94	49.90972	104.98	26.98	0.25000	0.89
1.64115	18.43	55.98482	40.35	32.88	0.50000	1.08
1.53385	45.52	60.28951	99.67	35.22	0.70000	4.72
1.42233	30.45	65.57999	66.68	27.92	0.35000	2.45

Data Sheet 3.10. Peak search and intensity data of XRD of 72.14% MnO_2 obtained by the chlorate treatment on fused $MnCO_3$.

Used wavelength:	K-Alpha1
K-Alpha1 wavelength (Å):	1.54056
K-Alpha2 wavelength (Å):	1.54439
K-Alpha2/K-Alpha1 intensity ratio:	0.50000
K-Alpha wavelength (Å):	1.54056
K-Beta wavelength (Å):	1.39222
Peak search parameter set:	**As Measured Intensities**
Set created:	2/21/03 13:11
Peak positions defined by:	Minimum of 2nd derivative
Minimum peak tip width (°2Theta):	0.00
Minimum peak tip width (°2Theta):	1.00
Peak base width (°2Theta):	2.00
Minimum significance:	0.60

d-spacing (Å)	Relative Intensity (%)	Angle (°2Theta)	Peak Height (counts/s)	Background (counts/s)	Tip Width (°2Theta)	Significance
3.01927	21.90	29.56156	16.07	36.72	0.60000	0.84
2.80586	28.20	31.86748	20.69	33.87	0.20000	0.61
2.40392	100.00	37.37744	73.36	49.04	0.40000	0.64
2.14820	45.83	42.02483	33.62	46.40	0.50000	0.66
1.84696	17.06	49.29737	12.51	36.22	0.80000	0.72
1.53153	17.35	60.39058	12.73	42.38	0.60000	0.63

Data Sheet 3.11. Peak search and intensity data of XRD of 80.60% MnO_2 obtained by HNO_3 treatment on fused $MnCO_3$.

Used wavelength:	K-Alpha1
K-Alpha1 wavelength (Å):	1.54056
K-Alpha2 wavelength (Å):	1.54439
K-Alpha2/K-Alpha1 intensity ratio:	0.50000
K-Alpha wavelength (Å):	1.54056
K-Beta wavelength (Å):	1.39222
Peak search parameter set:	**As Measured Intensities**
Set created:	2/21/03 13:11
Peak positions defined by:	Minimum of 2nd derivative
Minimum peak tip width (°2Theta):	0.00
Minimum peak tip width (°2Theta):	1.00
Peak base width (°2Theta):	2.00
Minimum significance:	0.60

d-spacing (Å)	Relative Intensity (%)	Angle (°2Theta)	Peak Height (counts/s)	Background (counts/s)	Tip Width (°2Theta)	Significance
4.76772	11.23	18.59509	8.23	13.70	0.30000	0.81
4.63711	10.19	19.12370	7.46	15.60	0.15000	0.61
3.02482	7.77	29.50610	5.69	25.57	0.30000	0.61
2.41211	100.00	37.24586	73.27	48.00	0.70000	3.75
2.11483	88.63	42.72014	64.94	28.55	0.10000	0.95
1.42560	19.56	65.41091	14.33	32.07	0.60000	1.04

Data Sheet 3.12. Peak search and intensity data of XRD of 74% MnO_2 obtained by the ozone treatment on fused $MnCO_3$.

Used wavelength:	K-Alpha1
K-Alpha1 wavelength (Å):	1.54056
K-Alpha2 wavelength (Å):	1.54439
K-Alpha2/K-Alpha1 intensity ratio :	0.50000
K-Alpha wavelength (Å):	1.54056
K-Beta wavelength (Å):	1.39222
Peak search parameter set:	**As Measured Intensities**
Set created:	2/21/03 13:11
Peak positions defined by:	Minimum of 2nd derivative
Minimum peak tip width (°2Theta):	0.00
Minimum peak tip width (°2Theta):	1.00
Peak base width (°2Theta):	2.00
Minimum significance:	0.60

d-spacing (Å)	Relative Intensity (%)	Angle (°2Theta)	Peak Height (counts/s)	Background (counts/s)	Tip Width (°2Theta)	Significance
2.44871	100.00	36.66912	56.16	41.14	0.30000	1.03
2.20478	21.74	40.89738	12.21	27.61	0.50000	0.74
2.15755	47.22	41.83416	26.52	28.07	0.60000	0.70
1.53699	21.83	60.15372	12.26	30.91	0.60000	0.68
1.43200	38.94	65.08203	21.87	34.46	1.00000	1.43