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X-RAY DIFFRACTION TO DETERMINE THE MINERALOGY IN SOIL SAMPLES IN THE UK

Heiam Hamed, William Hale, Ben Stern
 School of Archaeological and Forensic Sciences
 University of Bradford, UK

Abstract— Abstract in the soil samples collected for this study, the mineral composition present was identified using x-ray diffraction (XRD). The method used to identify the minerals was an automated search/match. From the results obtained from this method, all the peaks related to silica in the samples correspond to the silica in the database, while the calcite did not appear in the automated search. Therefore, a manual comparison was made by superimposing the reference XRD pattern over the measured XDR pattern. Silica, calcite and hematite were identified as present in all the soil samples.

Keywords— Soil, Mineralogy, X-Ray Diffraction, Determine minerals

I. INTRODUCTION

Similar to a human fingerprint, the diffraction pattern of each mineral has a specific X-ray reflection path [1]. For a single crystal, diffraction data are obtained from three dimensions. In powder diffraction, the data are obtained in a single dimension [2]. XRD is the best technique for identifying the inorganic materials by quantitatively analysing the minerals in soil and sediment [3]. Presently, XRD has been used in qualitative analysis more than in the quantitative analysis. For qualitative analysis crystalline phases with 25,000 organic components and 50,000 inorganic components have been measured as standards [4][5].

II. METHODOLOGY

A. Methods for data analysis –

The identification of minerals from X-ray powder diffraction is a 2-stage process [6]. The initial step is to compare the unknown XRD pattern of the sample to a reference mineral pattern by means of peak matching; however, XRD analysis of soil can often be problematic due to its complex nature as soil is composed of varying crystalline and amorphous components [7] The second step matches an unknown peak with a standard peak by comparing the 2-theta angle [8].

X-ray diffraction analysis is used in search or match procedures that help in comparing and identifying the determined peak using a database from numerous standards for different materials [9]. Minerals are identified by the process of manual searching, a method most commonly used in mineral

identification in the past which still has its benefits. It is beneficial for complex mixtures like soil or sediment samples in which diffraction peaks of crystalline phases are extremely weak [7]

B. Soil sample Preparation

This method follows that of Marathe et al. (2012). A hundred soil samples were collected across three sampling areas, Bradford, the area between Bradford/Leeds, and Leeds. Initially the soil samples were dried at room temperature to remove excess water. The sample holder, pestle and mortar were cleaned with ethanol, to reduce cross-contamination from other samples. Each soil sample was ground using a pestle and mortar until a fine powder was achieved, and the powder was put in the sample holder (silica wafer). Excess soil powder was removed utilizing a microscope glass slide and the surface was levelled. If the surface was not smooth and level, X-ray absorption would be possible and this reduces the intensity of small angle peaks [1] [11].

C. X-Ray Diffraction Meter Parameters

The soil samples were analysed by the method used by Linsen et al. (2014). A Bucker Axs D8 Advance X-ray diffractometer was used in this research. This instrument uses Bragg-Brentano geometry. The copper Ka X-ray source has a wavelength of 0.15406 nm. The voltage was 40kV while the filament emission was 30 mA. The samples were scanned over 2-theta and ranged from 5° to 50°. The intensity of the scattered X-ray was 3 seconds for every step where the step size was 0.003°. The X-ray beam covered the entire sample as a result of simultaneously scanning the sample in a rotation system.

In this case, the 2-theta value for different minerals has been obtained from previous studies which states that 2-theta and d-spacing for calcite, silica and hematite are as listed below in tables 4.1, 4.2, and 4.3 respectively.

2-THETA	D-SPACING
23.09	3.8526
29.44	3.0337
31.48	2.8416
36.02	2.4934
39.46	2.2834
43.22	2.0933



47.18	1.9263
47.58	1.9112
48.58	1.8742

Table 4.1: 2-theta and d-spacing for X-ray diffraction pattern of calcite [13].

2-THETA	D-SPACING
24.18	3.6806
33.2	2.6982
35.68	2.5164
39.34	2.2905
40.92	2.2056
43.57	2.0773
49.53	1.8403
54.15	1.6939

Table 4.2: 2-theta and d-spacing for X-ray diffraction pattern of hematite [14].

2-THETA	D-SPACING
20.88	4.2551
26.66	3.3432
36.58	2.4567
39.51	2.281
40.33	2.2365
42.49	2.1276
45.84	1.9797
50.19	1.8177

Table 4.3: 2-theta and d-spacing for X-ray diffraction pattern of silica [15].

III. RESULT AND DISCUSSION OF XRD PATTERN

Determining the Peak Location

Various factors are likely to shift the 2-theta peak positions from one sample to another [16]. Some of these factors include slight differences in automatic goniometer alignment, occasional alterations of the sample and inaccurately positioning the sample in the sample [16]. However, these factors do not affect the manual interpretation of the plots, but they complicate computerized mineral identification. According to Downs et al. (1993) it is possible to determine the type of mineral in a soil that contains a mixture of minerals using just two peaks (see also Dutrow 1997). Nanzyo et al. (2001) state that green and red lines respectively, while the black line shows the results for the soil sample in question.

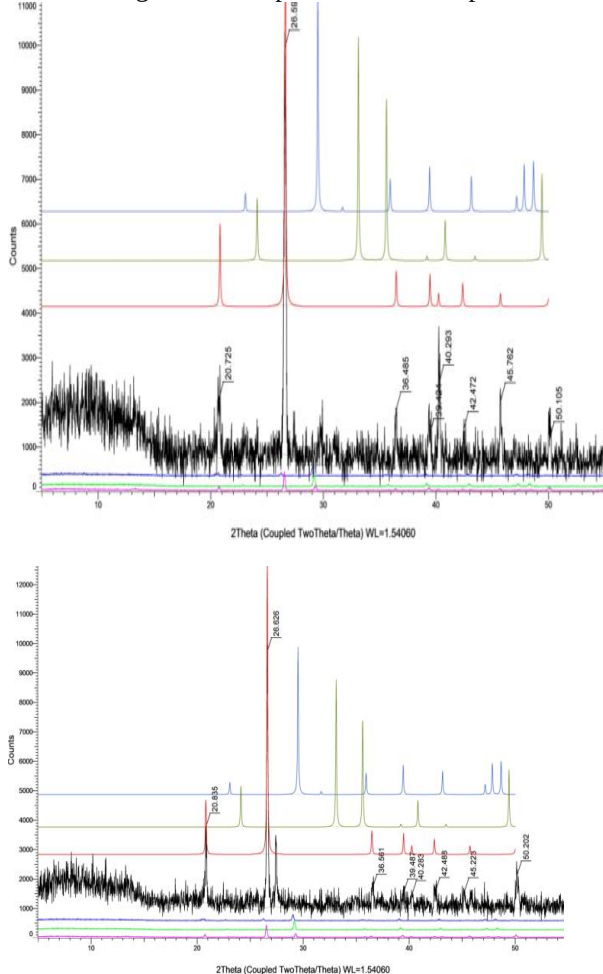
The 2-theta peaks for calcite in this case were at 23.09, 29.44, 31.48, 36.02, 39.46, 43.22, 47.18, 47.58 and 48.0. As can be seen in Figure.1a, a manual comparison of these peaks with the pattern in sample B1 shows that there was no match for most of these 2-theta values, although a match was found for values of 36.42 and 39.46. Therefore, according to Stewart (1966), this B1 sample does contain calcite. A similar comparison of the measured XRD pattern to the reference XRD pattern peak positions for hematite showed matches with only two 2-theta values of 24.17 and 39.46. By contrast there was matching of the sample pattern with most silica peak positions by this manual search method; an automated mineral search / match result is shown in Figure 4.1b, with a strong peak match Silica is therefore clearly indicated as being present in this sample distinction between these two peaks using the position of the peak is possible.

When it is difficult to determine a mineral from only using two or three peaks, then both the peak location and the d spacing values would be used to identify the mineral because each mineral has a unique combination of peak positions and d spacing values [19] The diffraction pattern for every phase is unique, so the XRD pattern for samples having the same peak can be solved by the difference in the d spacing values [20]. Phases with the same mineral composition can have drastically different diffraction patterns. The position of peaks to match experimental data to the reference patterns in the database to identify the mineral is done most precisely by profile fitting [17]. In this way, all the minerals in the soil can be determined using XRD.

In this study two minerals (silica and calcite) are selected in the laboratory to obtain a pattern of mixed minerals in different combinations. The reference peaks from the combinations of these minerals are then compared with the XRD results from the unknown samples to enable identification to be made. The technique is illustrated in this section for just two example samples, namely B1 and B2 taken from the Bradford area. In the present study, pure silica was mixed with pure calcite in varying proportions to create three standards, which were mixed as 1g silica with 1g calcite, 1g silica with 3g calcite and 3g silica with 1g calcite.

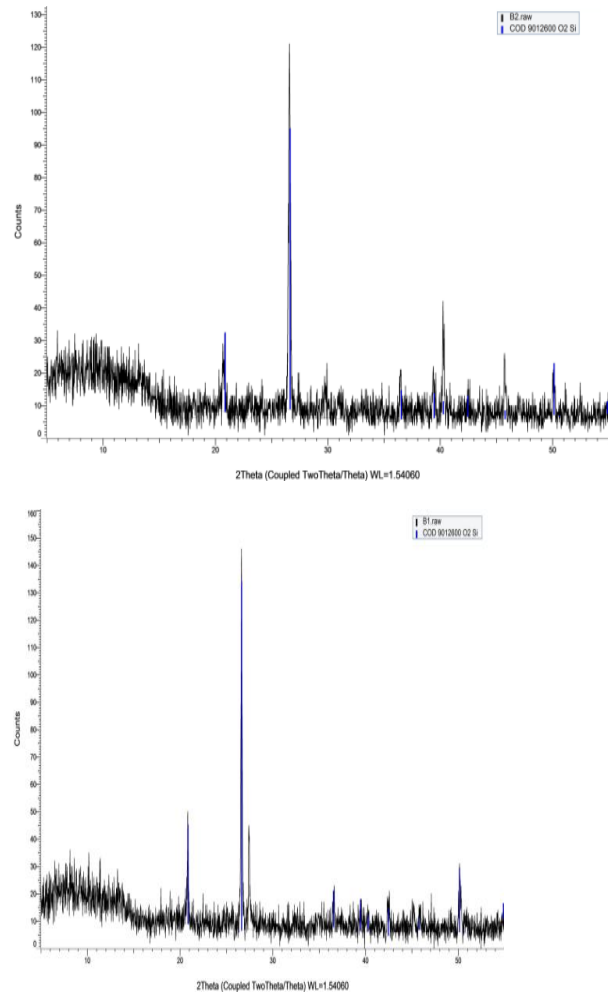
Figure.1a shows the results for the B1 sample. Use of the 1:1 silica: calcite, 1:3 silica: calcite and 3:1 silica: calcite standards enable the reference patterns for calcite, hematite and silica to be shown in Figure.1a by the blue, The results for sample B2 are shown in Figure.2. The XRD pattern for sample B2 only matched three peak positions for calcite corresponding to 2-theta values of 29.482, 36.40 and 39.478 (Figure.2a). Two 2-theta positions of 24.162 and 39.478 matched with hematite with a weak match, but are probably from hematite [17]. In Figure 3.23a the sample XRD patterns agreed with most silica peak positions, however the 2-theta value of 29.43 matches with calcite. In Figure.2a and Figure.2b the match for silica with all peaks found. It should be noted that samples including this

one may contain ‘noise’ (unexplained variation), which could be due to organic matter present in the sample.



(a)

Fig.1a: XRD pattern for sample B1 and XRD reference patterns for calcite (blue), hematite (green) and silica (red). Dark blue XRD patterns show 1g pure silica mixed with 1 g pure calcite, light green XRD patterns show mixed 1 g silica to 3 g calcite and pink XRD patterns show 3 g silica to 1g calcite. Fig.1b: XRD pattern for sample B1 by matching with silica using the XRD database.



(b)

Fig.2 a: XRD pattern for sample B2 and XRD reference patterns for calcite (blue), hematite (green) and silica (red) Dark blue XRD patterns show 1g pure silica mixed with 1 g pure calcite, light green XRD patterns show mixed 1 g silica to 3 g calcite and pink XRD patterns show 3 g silica to 1g calcite. Fig.2b: XRD pattern for sample B2 by matching with silica using the XRD database

Clearly all the areas of this study contain peaks which match with all the peaks of silica. However, calcite and hematite peaks do not always correspond with the reference pattern in three peak positions but sometimes only in two, possibly because the calcite interacts with the organic material present and covers the mineral which, according to Karine et al. (2005), prevents the correct interaction of the X-rays and the minerals so only certain peaks appear.

Calcium is a major, abundant metallic element, present at about 3.0% by weight in the Earth's upper continental crust and widespread in many minerals. However, in the UK, these occur mainly in the south and east of England, and the soils in these areas tend to have naturally high pH values. Very low Ca



concentrations are present over large areas of Wales, the Pennines, Cumbria, the North York Moors, Devon and Cornwall, the Hampshire Basin and the Weald of Kent and Sussex [22][23]. Silica minerals constitute more than 90% of the minerals in the Earth's crust. Silica minerals are grouped into six types based on the bonding structure of their silica

tetrahedrons [24]. The major primary minerals in soil are silica minerals. It is therefore to be expected that the soil samples analysed in the present study, taken from West Yorkshire in northern England away from any calcareous geology, would be high in silicates and low in calcium, as has indeed been found.

2-THETA / Calcite	B1	B2	B3	B4	B5	B6	B7	B8	B9	B10	B11	B12	B13	B14	B15	B16	B17	B18	B19	B20
23.09	23	23.1																		
29.44		29.48	29.46	29.5																
31.48	32																			
36.02	36	36.4	36.05	36.4	36.4	36.42	36.42	36.46	36.5	36.4	36.4	3.458	36.46	36.1	36.4	36.06	36.46	36.46	36.44	36.4
39.46	39	39.48	39.46	39.6	39.5	39.45	39.48	39.49	39.5	39.5	39.5	39.48	39.48	39.5	39.48	39.46	39.42	39.48	39.48	39.48
43.22																				
47.18																				
47.58																				
48.58																				
2-THETA / Calcite	B21	B22	B23	B24	B25	B26	B27	B28	B29	B30	B31	B32	B33	B34	B35	B36	B37	B38	B39	B40
23.09																				
29.44		29.46		29.5							29.4		29.48		29.48	29.47				
31.48																				
36.02	36	36.48	36.47	36.5	36.5	36.66	36.48	36.46	36.5	36.5	36.5	36.48	36.48	36.5	36.48	36.47	36.48	36.46	36.48	36.48
39.46	39	39.48	39.48	39.5	39.4	39.48	39.48	39.44	39.4	39.5	39.5	39.44	39.48	39.5	39.46	39.46	39.44	39.5	39.48	39.49
43.22																				
47.18																				
47.58																				
48.58																				

Table .4:. Presents the manually searched peaks matching with calcite reference patterns for samples from Bradford

2-THETA / Hematite	B1	B2	B3	B4	B5	B6	B7	B8	B9	B10	B11	B12	B13	B14	B15	B16	B17	B18	B19	B20
24.18		24.16	24.18	24.16	24.16	24.18	24.14	24.16	24.14	24.18	24.14	24.18	24.19	24.16	24.18	24.16	24.14	24.14	24.18	24.12
33.2																				
35.68																				
39.43	39.46	39.48	39.46	39.58	39.48	39.45	39.48	39.49	39.48	39.48	39.49	39.48	39.48	39.48	39.48	39.46	39.42	39.48	39.48	39.48
40.92																				
43.57																				
49.53																				
54.15																				
2-THETA / Hematite	B21	B22	B23	B24	B25	B26	B27	B28	B29	B30	B31	B32	B33	B34	B35	B36	B37	B38	B39	B40
24.18	24.16	24.18	24.1	24.18	24.18	24.18	24.18	24.16	24.16	24.18	24.12	24.16	24.18	24.16	24.16	24.16	24.14	24.12	24.18	24.16
33.2																				
35.68																				
39.43	39.48	39.48	39.48	39.48	39.44	39.48	39.48	39.44	39.42	39.46	39.46	39.44	39.48	39.46	39.46	39.46	39.44	39.5	39.48	39.49
40.92																				
43.57																				
49.53																				
54.15																				

Table .5: Presents the manually searched peaks matching with hematite reference patterns for samples from Bradford



2-THETA /silica	B1	B2	B3	B4	B5	B6	B7	B8	B9	B10	B11	B12	B13	B14	B15	B16	B17	B18	B19	B20
20.88	20.88	20.82	20.88	20.9	20.88	20.88	20.86	20.88	20.88	20.88	20.9	20.88	20.84	20.86	20.84	20.84	20.859	20.84	20.88	20.84
26.66	26.66	26.67	26.64	26.7	26.66	26.66	26.68	26.62	26.66	26.62	26.7	26.62	26.64	26.66	26.65	26.68	26.683	26.66	26.68	26.68
36.58	36.58	36.58	36.58	36.6	36.58	36.66	36.56	36.58	36.54	36.58	36.6	36.58	36.56	36.58	36.52	36.58	36.561	36.56	36.42	36.54
39.5	39.46	39.48	39.46	39.6	39.48	39.45	39.48	39.49	39.48	39.48	39.5	39.48	39.48	39.48	39.48	39.46	39.42	39.48	39.48	39.48
40.33	40.32	40.32	40.32	40.3	40.32	40.32	40.32	40.32	40.32	40.32	40.32	40.32	40.3	40.32	40.32	40.32	40.32	40.32	40.32	40.32
42.49	42.48	42.48	42.46	42.5	42.42	42.44	42.41	42.46	42.44	42.48	42.4	42.46	42.44	42.46	42.49	42.48	42.481	42.44	42.48	42.46
45.49	45.82	45.84	45.86	45.8	45.84	45.84	45.8	45.84	45.49	45.84	45.8	45.84	45.84	45.82	45.82	45.54	45.82	45.86	45.82	45.82
50.19	50.18	50.16	50.18	50.1	50.14	50.12	50.16	50.18	50.14	50.16	50.1	50.14	50.1	50.16	50.14	50.19	50.141	50.18	50.18	50.18
54.93	54.9	54.9	54.92	55	54.95	54.91	54.93	54.93	54.9	54.9	54.91	54.94	54.94	54.94	54.92	54.9	54.941	54.92	54.94	54.94

2-THETA /silica	B21	B22	B23	B24	B25	B26	B27	B28	B29	B30	B31	B32	B33	B34	B35	B36	B37	B38	B39	B40
20.88	20.88	20.88	20.88	20.9	20.88	20.86	20.88	20.84	20.88	20.9	20.8	20.88	20.86	20.86	20.84	20.86	20.88	20.88	20.88	20.88
26.66	26.66	26.66	26.6	26.7	26.64	26.67	26.66	26.68	26.66	26.68	26.7	26.68	26.68	26.68	26.66	26.66	26.64	26.66	26.66	26.66
36.58	36.46	36.56	36.56	36.6	36.54	36.56	36.54	36.52	36.58	36.58	36.6	36.58	36.56	36.57	36.52	36.54	36.5	45.94	36.56	36.56
39.5	39.48	39.48	39.48	39.5	39.44	39.48	39.48	39.44	39.42	39.46	39.5	39.44	39.48	39.46	39.46	39.46	39.44	39.5	39.48	39.49
40.33	40.32	40.32	40.32	40.3	40.32	40.32	40.32	40.32	40.32	40.32	40.3	40.32	40.32	40.32	40.32	40.32	40.32	40.32	40.32	40.32
42.49	42.48	42.46	42.47	42.4	42.44	42.46	42.48	42.44	42.4	42.42	42.4	42.48	42.49	42.46	42.46	42.48	42.44	42.48	42.48	42.48
45.49	45.8	45.84	45.84	45.9	45.8	45.86	45.82	45.82	45.8	45.82	45.8	45.82	45.44	45.8	45.84	45.82	45.82	45.84	45.82	45.84
50.19	50.16	50.12	50.16	50.2	50.14	50.14	50.18	50.18	51.17	50.16	50.2	50.14	50.17	50.14	50.17	50.18	50.18	50.18	50.18	50.18
54.93	54.92	54.92	54.9	54.9	54.96	54.94	54.9	54.92	54.96	54.9	54.9	54.9	54.9	54.92	54.94	54.92	54.95	54.94	54.92	54.93

Table .6: Presents the manually searched peaks matching with silica reference patterns for samples from Bradford.

2-THETA /Hematite	BL1	BL2	BL3	BL4	BL5	BL6	BL7	BL8	BL9	BL10	BL11	BL12	BL13	BL14	BL15	BL16	BL17	BL18	BL19	BL20
24.18	24.18																			
33.2		33.24	33.2	33.22	33.2	33.2	33.2	33.26	33.22	33.12	33.2	33.2	33.2	33.22	33.2	33.25	33.202	33.203	33.221	33.22
35.68																				
39.43	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46
40.92																				
43.57																				
49.53																				
54.15																				

Table .7: Presents the manually searched peaks matching with calcite reference patterns for samples from areas between Bradford/Leeds

2-THETA /Calcite	BL1	BL2	BL3	BL4	BL5	BL6	BL7	BL8	BL9	BL10	BL11	BL12	BL13	BL14	BL15	BL16	BL17	BL18	BL19	BL20
23.09								23.12												
29.44												29.44			29.46	29.44	29.48	29.47	29.46	
31.48																				
36.02	36.26	36.37	36.44	36.44	36.44	36.36	36.26	36.06	36.46	36.4	36.44	36.46	36.48	36.48	36.46	36.48	36.48	36.46	36.46	36.48
39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46
43.22																				
47.18																				
47.58																				
48.58																				

Table .8: Presents the manually searched peaks matching with hematite referent patents for samples from areas between Bradford/Leeds.

2THETA /silica	BL1	BL2	BL3	BL4	BL5	BL6	BL7	BL8	BL9	BL10	BL11	BL12	BL13	BL14	BL15	BL16	BL17	BL18	BL19	BL20
20.88	20.88	20.86	20.878	20.86	20.88	20.88	20.87	20.86	20.84	20.86	20.88	20.86	20.86	20.858	20.859	20.88	20.88	20.861	20.86	20.88
26.66	26.67	26.658	26.67	26.68	26.67	26.68	26.66	26.65	26.67	26.68	26.67	26.66	26.67	26.649	26.643	26.68	26.67	26.66	26.68	26.67
36.58	36.46	36.46	36.44	36.44	36.44	36.46	36.46	36.46	36.46	36.44	36.44	36.46	36.48	36.48	36.46	36.48	36.48	36.46	36.46	36.48
39.5	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46	39.46
40.33	40.32	40.32	40.32	40.32	40.32	40.32	40.32	40.32	40.32	40.32	40.32	40.32	40.32	40.32	40.32	40.3	40.3	40.35	40.32	40.32
42.49	42.46	42.44	42.441	42.48	42.44	42.47	42.48	42.46	42.46	42.48	42.42	42.44	42.459	42.48	42.46	42.46	42.48	42.439	42.478	42.46
45.49	45.48	45.48	45.46	45.42	45.48	45.46	45.44	45.46	45.44	45.46	45.44	45.46	45.48	45.48	45.48	45.48	45.467	45.4	45.48	45.48
50.19	50.18	50.17	50.18	50.18	50.18	50.16	50.16	50.16	50.18	50.18	50.12	50.16	50.15	50.183	50.16	50.157	50.118	50.179	50.259	50.18
54.93	54.92	54.9	54.9	54.92	54.9	54.9	54.92	54.94	54.92	54.92	54.94	54.92	54.94	54.94	54.944	54.9	54.909	54.94	54.919	54.94

Table .9: Presents the manually searched peaks matching with silica referent patents for samples from areas between Bradford/Leeds.



2-THETA /Calcite	L1	L2	L3	L4	L5	L6	L7	L8	L9	L10	L11	L12	L13	L14	L15	L16	L17	L18	L19	L20
23.09																				
29.44	29.44	29.46	29.46					29.42	29.44		29.46	29.46		29.483		29.46				29.46
31.48																				
36.02	36.54	36.46	36.46	36.48	36.47	36.46	36.48	36.46	36.48	36.46	36.48	36.46	36.46	36.46	36.46	36.68	36.44	36.48	36.46	36.5
39.46	39.4	39.46	39.46	39.4	39.46	39.46	39.46	39.46	39.46	39.48	39.48	39.47	39.47	39.46	39.46	39.46	39.46	39.46	39.47	39.46
43.22																				
47.18																				
47.58																				
48.58																				
2-THETA /Calcite	L21	L22	L23	L24	L25	L26	L27	L28	L29	L30	L31	L32	L33	L34	L35	L36	L37	L38	L39	L40
23.09																				
29.44	29.48			29.44		29.48			29.46	29.47	29.46		29.44		29.42					
31.48																				
36.02	36.46	36.46	36.48	36.4	36.46	36.42	36.46	36.46	36.44	36.46	36.22	36.46	36.48	36.44	36.46	36.46	36.48	36.48	36.44	36.58
39.46	39.46	39.47	39.46	39.46	39.46	39.46	39.46	39.46	39.44	39.46	39.46	39.46	39.46	39.44	39.46	39.46	39.46	39.44	39.46	39.46
43.22																				
47.18																				
47.58																				
48.58																				

Table.10: Presents the manually searched peaks matching with calcite reference patterns for samples from Leeds

2-THETA /Hematite	L1	L2	L3	L4	L5	L6	L7	L8	L9	L10	L11	L12	L13	L14	L15	L16	L17	L18	L19	L20
24.18	24.16	24.16	24.183		24.16	24.18	24.14	24.16		24.16	24.16	24.16	24.24	24.18	24.161	24.18				24.12
33.2									33.22		33.24									
35.68																				
39.43	39.4	39.46	39.46	39.4	39.46	39.46	39.46	39.46	39.46	39.48	39.48	39.47	39.47	39.46	39.46	39.46	39.46	39.46	39.47	39.46
40.92																				
43.57																				
49.53																				
54.15																				
2-THETA /Hematite	L21	L22	L23	L24	L25	L26	L27	L28	L29	L30	L31	L32	L33	L34	L35	L36	L37	L38	L39	L40
24.18	24.14	24.1			24.12	24.18	24.16		24.18	24.14	24.1	24.14			24.18					
33.2																				
35.68																				
39.43	39.46	39.47	39.46	39.46	39.46	39.46	39.46	39.46	39.44	39.46	39.46	39.46	39.46	39.44	39.46	39.46	39.46	39.44	39.46	39.46
40.92																				
43.57																				
49.53																				
54.15																				

Table.11.: Presents the manually searched peaks matching with hematite reference patterns for samples from Leeds.

2-THETA /silica	L1	L2	L3	L4	L5	L6	L7	L8	L9	L10	L11	L12	L13	L14	L15	L16	L17	L18	L19	L20
20.88	20.88	20.88	20.88	20.88	20.88	20.86	20.86	20.88	20.88	20.88	20.88	20.86	20.88	20.86	20.88	20.84	20.88	20.878	20.86	20.88
26.66	26.64	26.68	26.648	26.66	26.67	26.66	26.66	26.66	26.66	26.66	26.65	26.64	26.64	26.67	26.637	26.64	26.67	26.64	26.6	26.64
36.58	36.54	36.46	36.46	36.48	36.47	36.46	36.48	36.46	36.48	36.46	36.48	36.46	36.46	36.46	36.46	36.68	36.44	36.48	36.46	36.5
39.5	39.4	39.46	39.46	39.4	39.46	39.46	39.46	39.46	39.46	39.48	39.48	39.47	39.47	39.46	39.46	39.46	39.46	39.46	39.47	39.46
40.33	40.32	40.32	40.32	40.32	40.32	40.32	40.32	40.32	40.32	40.3	40.34	40.34	40.3	40.34	40.32	40.32	40.32	40.32	40.32	40.32
42.49	42.44	42.46	42.459	42.48	42.44	42.46	42.48	42.46	42.46	42.47	42.48	42.44	42.46	42.44	42.486	42.439	42.489	42.423	42.49	42.48
45.49	45.46	45.44	45.48	45.47	45.48	45.44	45.47	45.5	45.52	45.54	45.48	45.48	45.46	45.48	45.34	45.48	45.48	45.48	45.482	45.48
50.19	50.15	50.18	50.179	50.14	50.16	50.18	50.18	50.18	50.16	50.16	50.18	50.16	50.18	50.16	50.18	50.182	50.159	50.182	50.16	50.16
54.93	54.94	54.94	54.92	54.92	54.92	54.92	54.94	54.94	54.92	54.94	54.92	54.92	54.92	54.92	54.919	54.919	54.94	54.918	54.922	54.9
2-THETA /silica	L21	L22	L23	L24	L25	L26	L27	L28	L29	L30	L31	L32	L33	L34	L35	L36	L37	L38	L39	L40
20.88	20.84	20.88	20.88	20.67	20.86	20.88	20.86	20.86	20.88	20.84	20.88	20.84	20.86	20.86	20.88	20.79	20.88	20.88	20.86	20.8
26.66	26.66	26.66	26.66	26.66	26.68	26.66	26.67	26.66	26.66	26.66	26.68	26.66	26.61	26.67	26.65	26.65	26.64	26.67	26.65	26.66
36.58	36.46	36.46	36.48	36.4	36.46	36.42	36.46	36.46	36.44	36.46	36.22	36.46	36.48	36.44	36.46	36.46	36.48	36.48	36.44	36.58
39.5	39.46	39.47	39.46	39.46	39.46	39.46	39.46	39.46	39.44	39.46	39.46	39.46	39.46	39.44	39.46	39.46	39.46	39.44	39.46	39.46
40.33	40.32	40.32	40.32	40.3	40.32	40.3	40.32	40.32	40.32	40.32	40.32	40.32	40.32	40.32	40.32	40.32	40.32	40.32	40.32	40.32
42.49	42.48	42.48	42.43	42.48	42.46	42.44	42.48	42.48	42.46	42.46	42.44	42.44	42.48	42.48	42.48	42.46	42.48	42.46	42.48	42.46
45.49	45.52	45.42	45.48	45.48	45.42	45.42	45.44	45.48	45.48	45.48	45.48	45.46	45.4	45.46	45.4	45.48	45.48	45.42	45.48	45.48
50.19	50.12	50.12	50.18	50.16	50.14	50.18	50.16	50.18	50.18	50.18	50.18	50.15	50.16	50.16	50.19	50.19	50.16	50.17	50.18	50.18
54.93	54.94	54.92	54.92	54.94	54.92	54.92	54.95	54.94	54.95	54.95	54.9	54.94	54.91	54.94	54.94	54.96	54.9	54.92	54.92	54.12



Table .12: Presents the manually searched peaks matching with silica reference patterns for samples from Leeds

IV. CONCLUSION

One hundred soil samples were analysed by XRD to determine their mineralogical composition. Manual and automatic interpretation was used to determine the presence or absence in the soils of three minerals. Calcite, hematite and silica were identified in all soil samples; it was not possible to quantify the percentage values using this technique, but the mineralogical composition of all of the samples was clearly broadly consisting of the same components.

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