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Environmental Management - Grand Junction Office

UMTRA Project

Final Remedial Action Plan and Site Design for Stabilization of Moab Title I Uranium Mill Tailings At the Crescent Junction, Utah, Disposal Site

Attachment 4: Water Resource Protection

U.S. Department of Energy

Office of Environmental Management

Work Performed Under DOE Contract No. DE-AT30-07CC00014 and No. DE-AC01-02GJ79491
for the U.S. Department of Energy Office of Environmental Management.
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Remedial Action Plan and Site Design for Stabilization of Moab Title I Uranium Mill Tailings at the Crescent Junction, Utah, Disposal Site

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Calculation Cross-Reference Guide

Location	Calculation Number	Calculation Title
Attachment 1: Draft RAP Disposal Cell Design Specifications		
Appendix A	MOA-02-08-2006-5-19-01	Freeze/Thaw Layer Design
Appendix B	MOA-02-08-2006-5-13-01	Radon Barrier Design Remedial Action Plan
Appendix C	MOA-02-05-2007-5-17-02	Slope Stability of Crescent Junction Disposal Cell
Appendix D	MOA-02-05-2007-3-16-01	Settlement, Cracking, and Liquefaction Analysis
Appendix E	MOA-02-09-2005-2-08-01	Site Drainage – Hydrology Parameters
Appendix F	MOA-02-06-2006-5-08-00	Crescent Junction Site Hydrology Report
Appendix G	MOA-02-04-2007-5-25-02	Diversion Channel Design, North Side Disposal Cell
Appendix H	MOA-02-08-2006-6-01-00	Erosional Protection of Disposal Cell Cover
Appendix I	MOA-01-06-2006-5-02-01	Volume Calculation for the Moab Tailings Pile
Appendix J	MOA-02-08-2006-5-03-00	Weight/Volume Calculation for the Moab Tailings Pile
Appendix K	MOA-01-08-2006-5-14-00	Average Radium-226 Concentrations for the Moab Tailings Pile
Attachment 2: Geology		
Appendix A	MOA-02-04-2007-1-05-01	Site and Regional Geology – Results of Literature Research
Appendix B	MOA-02-04-2007-1-01-01	Surficial and Bedrock Geology of the Crescent Junction Disposal Site
Appendix C	MOA-02-04-2007-1-06-01	Site and Regional Geomorphology – Results of Literature Research
Appendix D	MOA-02-04-2007-1-07-01	Site and Regional Geomorphology – Results of Site Investigations
Appendix E	MOA-02-04-2007-1-08-01	Site and Regional Seismicity – Results of Literature Research
Appendix F	MOA-02-04-2007-1-09-02	Site and Regional Seismicity – Results of Maximum Credible Earthquake Estimation and Peak Horizontal Acceleration
Appendix G	MOA-02-04-2007-1-02-01	Photogeologic Interpretation
Attachment 3: Ground Water Hydrology		
Appendix A	MOA-02-02-2006-2-07-00	Saturated Hydraulic Conductivity Determination of Weathered Mancos Shale
Appendix B	MOA-02-03-2006-2-10-00	Field Permeability “Bail” Testing
Appendix C	MOA-02-03-2006-2-06-00	Field Permeability “Packer” Testing
Appendix D	MOA-02-04-2006-2-03-00	Hydrologic Characterization – Ground Water Pumping Records
Appendix E	MOA-02-05-2006-2-13-00	Hydrologic Characterization – Vertical Travel Time to Uppermost (Dakota) Aquifer
Appendix F	MOA-02-02-2007-3-01-00	Geochemical Characterization – Radiocarbon Age Determinations for Ground Water Samples Obtained From Wells 0203 and 0208
Appendix G	MOA-02-06-2007-2-14-00	Hydrologic Characterization – Lateral Spreading of Leachate
Attachment 4: Water Resources Protection		
Appendix A	MOA-02-06-2006-5-24-00	Material Placement in the Disposal Cell
Appendix B	MOA-02-06-2006-3-05-00	Geochemical Attenuation and Performance Assessment Modeling
Attachment 5: Field and Laboratory Results, Volume I		
Appendix A	MOA-02-03-2006-1-03-00	Corehole Logs for the Crescent Junction Site
Appendix B	MOA-02-03-2006-1-11-00	Borehole Logs for the Crescent Junction Site
Appendix C	MOA-02-03-2006-1-04-00	Geophysical Logs for the Crescent Junction Site
Appendix D	MOA-02-03-2006-1-10-00	Test Pit Logs for the Crescent Junction Site
Appendix E	MOA-02-03-2006-4-01-00	Geotechnical Properties of Native Materials
Appendix F	MOA-01-06-2006-5-22-00	Cone Penetration Tests for the Moab Processing Site
Appendix G	MOA-02-05-2006-4-07-00	Seismic Rippability Investigation for the Crescent Junction Site
Appendix H	MOA-02-03-2007-3-04-01	Background Ground Water Quality for the Crescent Junction Site
Appendix I	MOA-01-08-2006-4-08-00	Boring and Test Pit Logs for the Moab Processing Site
Appendix J	MOA-01-08-2006-4-09-01	Geotechnical Laboratory Testing Results for the Moab Processing Site
Appendix K	MOA-02-04-2007-4-03-01	Supplemental Geotechnical Properties of Native Materials
Attachment 5: Field and Laboratory Results, Volume II		
Appendix L	MOA-02-08-2006-1-06-00	Compilation of Geologic and Geophysical Logs
Appendix M	N/A	Radiological Assessment for Non-Pile Areas of the Moab Project Site
Appendix N	MOA-02-05-2007-4-04-00	Supplemental Geotechnical Properties of Tailings Materials from the Moab Processing Site

Attachment 4
Table of Contents

Appendix A Material Placement in the Disposal Cell
Appendix B Geochemical Attenuation and Performance Assessment Modeling

U.S. Department of Energy—Grand Junction, Colorado

Calculation Cover Sheet

Calc. No.: MOA-02-06-2006-5-24-00 **Discipline:** Construction **No. of Sheets:** 4
Doc. No.: X0173600

Location: Attachment 4, Appendix A

Project: Moab UMTRA Project

Site: Crescent Junction Disposal Site

Feature: Material Placement in the Disposal Cell

Sources of Data:

UMTRA Specifications, Earthwork, Section 02200, Revision 15, Document Number 5025-GRJ-S-01-01029-17

Sources of Formulae and References:

None.

Preliminary Calc. ☐ **Final Calc.** ☒ **Supersedes Calc. No.**

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Problem Statement:

Develop a placement methodology that allows the residual radioactive material to be placed in the cell in manner that is efficient for construction but does not cause excessive or differential settlement or provide conditions that would cause the tailings to be susceptible to liquefaction. In addition, the placement method must be able to handle the oversized material and debris that must be disposed of in the cell.

Method of Solution:

The UMTRA program has successfully constructed and disposed of residual radioactive material and debris in 22 disposal cells. Utilizing the same method is warranted at this site.

Assumptions:

Existing specification incorporates lessons learned during a multiple-year, multiple-site project and is relevant for the work in Moab.

Calculation:

Not Applicable. See Discussion section.

Discussion:

Sample Material Placement Specification

- No material shall be placed on any portion of the subgrade or against any berm until consent to place fill is obtained from the Contractor.
- Material shall not be placed on frozen subgrade or frozen material, nor shall frozen material be placed in the cell for final placement.
- Material shall be placed to maintain positive drainage and to prevent ponding. Prior to forecast precipitation events, the subcontractor shall roll or back-blade material to provide a compacted surface that promotes runoff.
- Fill materials shall be placed in continuous and approximately horizontal lifts for their full length and width unless otherwise specified or specifically permitted by the Contractor.
- Method of dumping and spreading of material shall ensure uniform distribution of material and prevent segregation.
- Loose thickness of each lift of materials shall not be greater than that required to achieve the specified compaction. In no case shall the lift thickness exceed 12 inches, except in cases of backfilling around debris that requires thicker lifts.
- Material shall be placed and compacted to a density of at least 95 percent of Standard Proctor maximum dry density and -3 percent to +2 percent of optimum moisture content.
- Wet materials may be disked, blended, scarified, plowed, or air-dried in order to meet required moisture content. Dry materials may need to be blended with wetter materials or be wetted to meet the required moisture content.
- Materials that have been placed and compacted that are outside the range of either density or moisture content shall be re-worked until the materials meet the requirements.
- Disposal of oversized material (greater that 6 inches in any direction) and debris shall be done evenly in the embankment to minimize the voids created. Material shall be spread out to promote compaction of material in the voids and to prevent nesting. Debris shall be disposed of at least 10 feet (ft) below the bottom of the radon barrier.

- Debris shall be no greater than 10 ft in any dimension and no greater than 27 cubic ft in volume. The autoclaves may be placed intact. Subcontractor shall provide a Work Plan describing loading, unloading, movement, placement, and placement of soil material around the autoclaves. All other material shall be size-reduced to the maximum dimensions stated.
- Loads of debris shall be placed at least 15 ft apart.
- Large amounts of debris/trash that cannot be sized should be evenly spread.
- Loads of debris shall have at least 5 ft of separation vertically.
- Wide drains (geotextile material) do not need to be sized.
- Temporary toe drains, pumps, and piping shall be installed, operated, and maintained at the low end of the cell to remove construction water, precipitation runoff, and pore water until directed by the Contractor.

Field Quality Control

- Subcontractor will take samples and perform quality-control tests throughout the construction period in conformance with the Contractor-approved quality-control plan. Contractor may observe quality-control tests and will perform quality assurance tests. Subcontractor shall provide safe access for quality assurance tests and shall provide timely test data and any required assistance to the Contractor.
- In-place density and moisture-content tests shall be performed at a minimum of one test per 1000 cubic yards of material placed.
- There shall be a minimum of one in-place density and moisture content test performed on each shift of material placement.
- There shall be a minimum of one in-place density and moisture content test performed on each lift of material placement
- Locations of in-place density and moisture content tests shall be surveyed for northing, easting, and elevation. Locations shall be plotted and reported.

Conclusion and Recommendations:

Additional detail will be provided in final specifications.

Computer Source:

Not applicable.

U.S. Department of Energy—Grand Junction, Colorado

Calculation Cover Sheet

Calc. No.: MOA-02-06-2006-3-05-00 Discipline: Geochemical Properties No. of Sheets: 40
Doc. No.: X0173400

Location: Attachment 4, Appendix B

Project: Moab UMTRA Project

Site: Crescent Junction Disposal Site

Feature: Geochemical Attenuation and Performance Assessment Modeling

Sources of Data:

Sources of Formulae and References:

List of actual references reviewed.

Preliminary Calc. ☐ Final Calc. ☒ Supersedes Calc. No.

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Crescent Junction Disposal Site
Geochemical Characterization of Mancos Shale and Reaction-Transport Modeling of Contaminant Attenuation

Executive Summary

The purpose of this work was to develop a robust one-dimensional reaction-transport model that could be used by site personnel to help evaluate the attenuation of contaminants in ground water that may migrate from a proposed uranium mill tailings disposal cell at Crescent Junction, Utah. Although it is unlikely that contaminated water from the disposal cell will penetrate the thick Mancos Shale, contaminant attenuation by bedrock affords increased protection for deep ground water systems. Data for the model were derived from laboratory characterization of the bedrock beneath the proposed disposal cell. The disposal cell will contain tailings from the Moab, Utah, (Atlas) uranium mill and is underlain by the Mancos Shale. Samples of Mancos Shale were collected from 10 cores that were evenly distributed in the area of the proposed disposal cell. Five samples were collected from each of the 10 cores for a total of 50 samples, at depths of 40 to 300 feet (ft).

The chemistry of the water-soluble fractions of the samples was determined and used to help estimate the proportions and types of water-soluble minerals. Based on these results it is estimated that the water-soluble mineral assemblage is dominated by nahcolite ($NaHCO_3$) with major amounts of calcium (Ca) - sodium (Na) exchange and gypsum ($CaSO_4 \cdot 2H_2O$). Halite, sylvite, and dolomite occur in lesser amounts and calcite is present. Gypsum and dolomite are more dominant in the shallow samples, while nahcolite and halite are more concentrated in the deeper samples. The mineral abundances were used as initial conditions for the ground water reaction-transport model.

Cation exchange capacity (CEC) was measured on 20 core samples of Mancos Shale. CEC ranged from 0.54 to 36.29 milliequivalents per 100 grams (meq/100 g) with a mean of 11.23 meq/100 g. These values are consistent with shale composed of kaolinite, illite, and smectitic interlayered clay minerals as determined by x-ray diffraction analysis. In the reaction-transport modeling, the mean CEC value is used to specify the number of cation exchange sites. Cation exchange was used to model retardation of ammonium (NH_4).

X-ray diffraction (XRD) analysis on 10 samples of Mancos Shale was used to further identify minerals present in the core samples. The bulk mineralogy is dominated by quartz, with lesser amounts of dolomite and calcite, small amounts of feldspar, and traces of gypsum. The clay mineral fraction is dominated by mixed-layer (mostly illite/smectite) clays, illite, and kaolinite, with illite layers dominating the mixed-layer clays. The mineralogy was used to help estimate initial mineral composition for the reaction-transport model.

Particle surface area was determined by the standard Brunauer, Emmett, and Teller (BET) analysis on 10 Mancos Shale samples. Surface areas range from 8.81 to 13.22 square meters per gram (m^2/g) with a mean of 11.02 m^2/g. Surface area measured on a powdered split is consistent with surface areas measured on the 1- to 2-millimeter (mm) fractions, indicating that the BET method is probably accounting for intraparticle surface area. Surface area was used as an input to the surface-complexation adsorption algorithm in the reaction-transport model.

Distribution ratios (R_d) are a measure of the partitioning of a contaminant between the ground water and the solid fraction of the aquifer. The higher the R_d, the more partitioning to the solids and the more retardation of the contaminant. The R_d value can vary significantly with solution chemistry. For example, Davis et al. (2004) showed that R_d values for uranium in a sample of alluvium varied by more than a factor of 10 depending on dissolved carbonate concentration and pH value. For the reaction-transport modeling, a surface-complexation approach is used instead of using constant R_d values to simulate retardation of uranium (U). Using the surface-complexation approach, the R_d value changes as chemical conditions (especially pH and pCO_2) change in the aquifer. The results of the R_d determinations were complicated by the analytical imprecision associated with relatively small concentration differences between tests containing sediment and controls without sediment. However, the data indicate that R_d values for uranium adsorption on Mancos Shale are relatively low, ranging from essentially 0 to 0.84 milliliters per gram (mL/g).

The main use of the R_d values was to test and calibrate the surface-complexation module used for U transport in the reaction-transport modeling.

Two sequential batch-leaching tests were conducted to observe chemical evolution of tailings leachate as it interacted with Mancos Shale. One test simulated vertical transport and the other horizontal transport through the Mancos Shale. Chemical changes that occurred in the tailings leachate as it reacted with progressively more Mancos Shale in the horizontal simulation include slightly increasing values of alkalinity (pH), chloride (Cl), potassium (K), Na, sulfate (SO_4), and uranium (U). Similar to the simulation of horizontal transport, pH values in the vertical simulation progressively increased with increased reaction. Progressive increases also occurred in the Cl, Na, SO_4, and U concentrations, but decreasing trends in alkalinity and possibly NH_4 occurred. The results of the sequential batch tests were used to help calibrate the reaction-transport models.

The laboratory data discussed above were used to develop a one dimensional reaction-transport model of tailings fluid interaction with the Mancos Shale to simulate transport of contaminants beneath the Crescent Junction disposal cell. Two simulations were run, one simulation representing horizontal flow through shallow Mancos Shale and the other representing vertically downward flow through progressively deeper Mancos Shale. The only difference in input parameters between the horizontal and vertical simulations is the initial abundances of minerals, the deeper Mancos Shale having more nahcolite and less gypsum than the shallow Mancos Shale. The simulations were calculated with the transport algorithm embedded in the PHREEQC geochemical computer program.

In both the horizontal and vertical transport simulations, NH_4 is retarded for about 3.5 pore volumes, after which concentrations rise rapidly to the influent concentration. Retardation of NH_4 was caused by the exchange of dissolved NH_4 cations for solid-phase exchangeable Ca, K, Mg, and Na. Most of the exchange involves Na ion because Na dominates the cations in Mancos Shale ground water at the Crescent Junction Site. Effluent U concentrations in the horizontal simulation are retarded for slightly less than one pore volume during which the U concentration is less than about 0.075 mg/L. After one pore volume, U concentrations increase rapidly and reach the influent value (4 mg/L) after about 3 pore volumes. In the vertical simulation, U concentrations are never less than 2.4 mg/L; however, U concentrations remain less than the influent until about 4 pore volumes. In the horizontal simulation, distribution coefficient (K_d) values were initially 0.26 mL/g and decreased to 0.19 mL/g after about 2 pore volumes. In the vertical simulation, K_d values were negligible initially and increased to 0.15 mL/g after about 4 pore volumes. The differences in K_d values and dissolved U concentrations between the two simulations result from variation in the ionic composition of the solutions resulting from equilibration with minerals and cation exchange sites. A critical factor was the presence of a higher concentration of gypsum in the horizontal simulation than in the vertical simulation. Calcium released from dissolution of gypsum in the horizontal simulation caused precipitation of calcite, which resulted in decreased pH. These conditions led to increased partitioning of U to the specific adsorption sites on the Mancos Shale and increased retardation in the horizontal simulation.

In summary, the transport results suggest that NH_4 migration is retarded by several pore volumes. Uranium is retarded by about 1 pore volume, but only if Ca is released from gypsum dissolution. To evaluate the effects of this analysis on contaminant transport beneath the proposed Crescent Junction disposal cell, it is necessary to know the flux of contaminated water from the cell. The effective porosity of the Mancos Shale must also be known; attenuation would be much less in a system dominated by fracture flow than one dominated by porous media flow. Evaluation of the flow regime was beyond the scope of this investigation; thus, results of the model simulations are provided in terms of pore volumes. To maximize the benefit of these results in the field setting, project personnel will need to couple these results with results of hydrologic investigations to convert units of pore volume to more useful units of travel time and distance. Alternatively, a sensitivity analysis that uses reasonable bounds for the hydrologic parameters may be appropriate to assess the impact of chemical attenuation at the Crescent Junction Site.

Much of the work herein on U adsorption was developed recently by Dr. James Davis and co-workers at the U.S. Geological Survey. Work by Davis et al. was funded by the U.S. Nuclear Regulatory Commission (NRC) specifically to advance the state-of-the-art in geochemical methods used for the transport of U at uranium milling sites. Their model of surface complexation adsorption is well suited to the work presented here.

Introduction

This work was done to characterize the geochemistry of the bedrock beneath and adjacent to the proposed disposal cell location at Crescent Junction, Utah. The disposal cell will be constructed to contain tailings from the former Moab, Utah, (Atlas) uranium ore processing mill and will be underlain by the Mancos Shale. The purpose of this work is to provide data to help evaluate the potential for ground water contamination and transport of tailings constituents at the disposal site. The basis for this work is provided in Section 4.5 of the "Work Plan for Characterization of Crescent Junction Disposal Site" (Appendix A) and was modified based on discussions with Moab Uranium Mill Tailings Remedial Action (UMTRA) Project personnel. The scope, which includes laboratory investigations and reaction-transport modeling, is defined in Appendix A.

The geochemical approach involves collecting site-specific data and using these data to model geochemical interactions between tailings pore fluid and the Mancos Shale. Results of the laboratory investigations provide the following information about the Mancos Shale: (1) abundance and mineralogy of water-soluble minerals; (2) mineralogy of water-insoluble minerals, including clays; (3) cation exchange capacity (CEC); (4) surface area; and (5) chemical distribution ratios (R_d). These data were used to construct a one-dimensional reaction-transport model of tailings water transport through the Mancos Shale. The model includes equations governing aqueous speciation, mineral dissolution, mineral precipitation, mixing with other ground water, cation exchange, and adsorption. In addition, two sequential batch-leaching tests were conducted, and the results were used to help calibrate the geochemical model. Numerous analyses of tailings pore fluids have been made previously, and no additional analyses were made for this study.

Samples of Mancos Shale were collected from 10 cores that were evenly distributed in the area of the proposed disposal cell (see Appendix A for locations). Samples were obtained from the Prairie Canyon and Blue Gate Shale Members of the Mancos Shale, the geologic units that directly underlie the proposed disposal cell (Table 1). Five samples were collected from each of the 10 cores for a total of 50 samples. The disposal cell excavation will extend approximately 20 feet (ft) below the ground surface; thus, the uppermost sample of each core was collected from a depth of 40 ft. The remaining four samples per core were collected at equal intervals below 40 ft; with the deepest samples obtained at 300 ft. Evaluation of these samples provided a reasonable set of data to assess lateral and vertical distributions of geochemical properties in the Mancos Shale underlying the location of the proposed disposal cell.

Table 1. Geologic Members of Mancos Shale in Samples Used in This Study[a]

Boring Number	40-ft Depth	105-ft Depth	170-ft Depth	235-ft Depth	300-ft Depth
CJ-201	PC	PC	BG	BG	BG
CJ-202	BG	BG	BG	BG	BG
CJ-203	PC	PC	BG	BG	BG
CJ-204	PC	BG	BG	BG	BG
CJ-205	BG	BG	BG	BG	BG
CJ-206	PC/BG	BG	BG	BG	BG
CJ-207	BG	BG	BG	BG	BG
CJ-208	PC	PC	BG	BG	BG
CJ-209	BG	BG	BG	BG	BG
CJ-210	PC	PC	BG	BG	BG

[a]PC = Prairie Canyon Member. BG = Blue Gate Shale Member.

The water-soluble chemistry of all 50 samples was measured. Samples from the 40-ft depth (and some from the 105-ft depth) were used for additional analyses because these samples are representative of rock directly beneath the proposed tailings disposal cell and are most likely to contact migrating tailings fluids. All 40-ft-deep samples were analyzed for surface area, mineralogy by X-ray diffraction (XRD), CEC, and uranium (U) distribution ratios. In addition, all 105-ft-deep samples were measured for U, uranium $R_{d,}$ and CEC values.

This report is divided into 10 sections. Section 1.0 describes the general methods used for acquisition of samples and analyses. Sections 2.0 through 6.0 present methods and results for each characterization activity, and Section 7.0 provides the laboratory results of two sequential batch-leaching tests. Section 8.0 develops each module of a reaction-transport model and presents reaction-transport simulations for the sequential batch-leaching tests and the Crescent Junction Site. Section 9.0 gives the conclusion, and Section 10.0 lists the references.

Much of the U adsorption work presented herein uses an approach recently developed by Dr. James Davis and co-workers at the U.S. Geological Survey. Davis and Curtis (2003) present a sophisticated method to evaluate U adsorption using detailed data collected at a former uranium milling site at Naturita, Colorado, a site administered by the U.S. Department of Energy (DOE) Office of Legacy Management. The NRC funded the recent work by Davis and others specifically to advance the state-of-the-art in geochemical methods used for the transport of U at uranium milling sites.

1.0 General Methods

1.1 Sample Collection and Preparation

Five samples were collected from each of the 10 cores. The samples were collected at depths of 40, 105, 170, 235, and 300 ft. Sample numbers are in the format CJ-201-40, where CJ is Crescent Junction, 201 is the boring number, and 40 is the depth measured in feet. Samples were 2 inches in diameter and contained approximately 2.5 linear inches of core. Samples were air dried and stored in plastic containers until used for the tests. Dried samples were lightly crushed with a hammer or pestle, sieved, and split using a riffle splitter as needed for the tests. Bulk sample weights ranged from 238 grams (g) to 615 g. Moisture contents range from 0.76 percent to 3.01 percent and have no obvious relationship to sample depth or lithology. Laboratory notes are presented in Appendix B and a complete set of raw data and Excel calculations are presented in Appendix C.

1.2 Analytical Methods

The laboratory portion of the work was conducted in the DOE Environmental Sciences Laboratory at Grand Junction, Colorado. A subcontract was procured with Dr. William Hood, Grand Junction, Colorado, to conduct XRD analysis. Micromeritics Analytical Services, Norcross, Georgia, measured particle surface areas using the standard BET method. Table 2 presents analytical methods used for water chemistry measurements.

Table 2. Analytical Methods

Constituent	Procedure Number DOE (STO 210)	Procedure Description
Alkalinity	AP (Alk-1)	Titration with H_2SO_4
Ammonia	AP (NH_3-1)	Spectrometry-Salicylate
Calcium	AP (Ca-1)	Flame Atomic Absorption
Chloride	AP (Cl-2)	Ion Chromatography
Magnesium	AP (Mg-1)	Flame Atomic Absorption
Nitrate	AP (NO_3-4)	Ion Chromatography
Oxidation-Reduction Potential (ORP)	AP (ORP-1)	Electrode
pH	AP (pH-1)	Electrode
Potassium	AP (K-1)	Flame Atomic Absorption
Sodium	AP (Na-1)	Flame Atomic Absorption
Specific Conductance	AP (EC-1)	Electrode
Sulfate	AP (SO_4-4)	Ion Chromatography
Uranium	AP (U-2)	Kinetic Phosphorescence

2.0 Analysis of Water-Soluble Extracts

2.1 Introduction

This portion of the work scope was designed to identify and estimate abundances of minerals present in the water-soluble fraction of the Mancos Shale. The water-soluble fraction is the most reactive portion of the aquifer and will likely have a significant effect on chemical evolution of the ground water system. Appendix C contains a complete set of chemical results for the water-soluble extractions.

2.2 Methods

Samples were crushed, air dried, and sieved to –10 +18 mesh (1 to 2 mm nominal diameter). This size fraction was selected because it (1) is likely to have sufficient material to accomplish the tests, (2) is uniform enough so that surface area is relatively constant and easy to determine, (3) is efficient to work with in the laboratory (testing apparatus can be relatively small), and (4) should be reasonably representative of the bulk rock encountered in the field.

The leaching procedure was modified from procedure CB (BT-1) (STO 210). Two grams of the sieved sample was placed in a plastic centrifuge tube with 100 milliliters (mL) of deionized water at room temperature. The tube was agitated end over end for 4 hours. The solids were separated from the water by centrifuging and decanting to produce a clear solution. The solutions were analyzed for pH, oxidation-reduction potential (ORP), specific conductance, alkalinity, ammonium (NH_4), calcium (Ca), chloride (Cl), magnesium (Mg), nitrate (NO_3), potassium (K), sodium (Na), sulfate (SO_4), and U.

2.3 Results and Discussion

All 50 samples were analyzed by the water-extraction method. Analyses included major ions that constitute most water-soluble minerals as well as the mill tailings contaminants NH_4 and U. Mass balance calculations made using the computer program NETPATH (Plummer et al. 1994) were used to estimate the mineralogy of the water-soluble fraction. Mineral identifications were aided by XRD analyses (Section 4.0), but XRD is limited in its ability to detect small amounts (typically less than 10 percent) of minerals and does not provide quantitative information on mineral abundance. This section reports the concentrations of the constituents in the water-soluble fractions of the Mancos Shale samples and the mineral assemblages calculated using NETPATH.

2.3.1 Masses of Constituents in the Water-Soluble Extracts

The solid-phase concentration of each constituent (Table 3) was calculated from the measured concentration and the solids-to-solution ratio (2 g in 100 mL). The total water-soluble fraction ranged from 0.40 to 2.85 percent (by weight) of the sample, with a mean value of 0.72 percent (Table 3; 1 percent is equivalent to 1,000 micrograms per gram [µg/g]). Only two samples (CJ-203-40 and CJ-204-40) exceeded 1 percent, and both were from the 40-ft depth. Values of pH in the solutions after agitation ranged from 6.17 to 9.88, with a mean pH value of 9.50. Only five samples, all from the 40-ft depth, had pH values less than 9.00.

The water-soluble fractions are dominated by carbonate (alkalinity), Na, and SO_4, with lesser amounts of Ca, Cl, K, and Mg (see “Mean” in Table 3). Data in Table 3, show that Ca and SO_4 are more dominant in the shallow (40-ft) samples than in the samples obtained from deeper depths, suggesting the presence of more gypsum ($CaSO_4 \cdot 2H_2O$) in the shallow horizon. Alkalinity and Na appear to increase in the deeper horizons, suggesting the presence of nahcolite ($NaHCO_3$) in the deeper horizons.

Concentrations of NO_3-N were less than the detection limit of 5.5 µg/g in all but three samples. The three samples with higher NO_3-N values were collected at the 40-ft depth. Ammonia as N (NH_3-N) values ranged from less than the detection limit of 4 µg/g to 36 µg/g and had no obvious correlation with depth. Water-soluble U concentrations ranged from 0.006 to 0.519 µg/g. Only one sample (CJ-208-40) had a U concentration more than 0.1 µg/g, and that sample was from the 40-ft depth. These U values are low compared to an average total concentration of U reported for the Earth’s crust (1.8 µg/g; Mason and Moore 1982) and an average value (20 µg/g) reported by Wedepohl (1974) for marine black shale such

as the Mancos Shale. Part of the reason for the lower results is that the literature crustal and marine black shale averages were analyzed on total digestions of the rock rather than the water-soluble fractions.

2.3.2 Mineralogy of the Water-Soluble Fraction

The geochemical computer program NETPATH was used to calculate possible mineral assemblages dissolved from the Mancos Shale samples by the deionized water. The most common use of NETPATH is to model mineral-phase reactions that could occur as ground water flows through an aquifer, based on the water chemistry data of two ground water samples collected along a flow path. In this study, we used NETPATH to help evaluate the mineralogy of the water-soluble fractions. To do this, deionized water was used as the initial solution composition and the analytical results of the water after reaction with solid samples was used as the final water composition. Water-soluble concentrations of NH_3 and U were also measured, but the identification of the mineral phases containing these constituents was not pursued because of low concentrations of these contaminants. Results of XRD analysis helped to identify mineral phases that are most likely to contain the water-soluble components (Section 4.0).

Primer on NETPATH

To run NETPATH, the solution chemistry is entered into a database. From the database, dissolved species, mineral saturation indices, dissolved inorganic carbon concentration (from alkalinity), and electrical balance were calculated for each solution. The molal concentrations of the constituent elements were then imported to NETPATH for mass balance calculations. Combinations of mineral phases were specified, and the program calculated the amount of each phase that must precipitate or dissolve to meet the compositional constraints.

NETPATH solves a set of mass balance chemical equations and can determine a set of mineral assemblages to account for the chemical differences between two water compositions. For example, if water A has 10 millimoles (mmol) of Ca and evolves to water B that has 2 mmol of Ca, then 8 mmol of Ca was lost. Several chemical processes can account for the loss, including (1) precipitation of calcite ($CaCO_3$), (2) precipitation of gypsum, (3) exchange of Ca for Na on an exchanger, and other processes. Clearly, each process will produce other changes in the water chemistry; for example, calcite precipitation will cause carbon (C) loss, gypsum precipitation will cause SO_4 loss, etc. Thus, NETPATH models for this example are also constrained by mass balances for C and SO_4.

The user selects *constraints* and *permissible phases* for use with a simulation. *Constraints* are elements and *permissible phases* are minerals, exchange sites, or gases. Given the number of *constraints*, there must be enough *permissible phases* to afford a solution and there must be a phase for each *constraint* (for example if Ca is a *constraint*, there must be a phase that contains Ca).

Important points to remember about NETPATH models are (1) models are not unique, (2) models are not supported by thermodynamic principles (for example, a NETPATH model can have calcite precipitating, even though precipitation is impossible because of undersaturation), (3) the final water composition must have evolved from the initial composition (e.g., two water samples from the same stream tube in a flow system or water reacted with rock in a laboratory batch test such as was done in this study), and (4) the models are strongly a function of the *constraints* and *permissible phase*s selected by the user. The user selects *constraints* and *permissible phases* by evaluating the data available about the site and applying geochemical principles.

Table 3. Results of Water Extractions Expressed as Micrograms of Constituent Per Gram of Rock

Sample	pH	Alk	Cl	NO_3-N	SO_4	NH_3-N	U	Ca	Na	Mg	K	Total
CJ-201-40	7.97	450	399	10.95	3964	5.5	0.014	695	1040	170	485	7219
CJ-202-40	9.26	1800	494	25.73	816	6	0.047	22.5	1000	38	755	4957
CJ-203-40	6.17	600	159	15.24	20645	10	0.065	6120	450	400	100	28499
CJ-204-40	8.46	750	137	<5.50	8552.5	21	0.071	1840	1300	350	106	13062
CJ-205-40	9.16	1850	231	<5.50	785.5	20	0.073	12.5	1225	18.5	325	4473
CJ-206-40	8.78	1750	259	<5.50	1111.5	11.5	0.050	62.5	1075	36	115	4426
CJ-207-40	9.64	4050	210	<5.50	1492	36	0.040	4.5	2500	7	240	8545
CJ-208-40	9.29	1600	322	<5.50	835.5	7.5	0.519	52.5	1050	19	80	3972
CJ-209-40	8.49	1000	123.5	<5.50	4098.5	<4	0.043	250	1550	180	195	7407
CJ-210-40	9.72	3650	249.5	<5.50	780	16.5	0.041	9.5	1900	6.5	155	6773
CJ-201-105	9.39	1950	344	<5.50	366.5	4	0.010	38	1200	8	140	4056
CJ-202-105	9.78	4150	868.5	<5.50	216	16.5	0.035	9	1800	6	860	7932
CJ-203-105	9.52	2450	886.5	<5.50	377	13	0.055	22.5	1450	6.5	815	6026
CJ-204-105	9.85	4350	261	<5.50	254.5	17.5	0.055	5	2000	5.5	280	7179
CJ-205-105	9.73	4650	369	<5.50	330	23.5	0.041	3	2050	6	230	7667
CJ-206-105	9.29	2200	322.5	<5.50	429.5	14.5	0.011	34.5	1150	39.5	110	4306
CJ-207-105	9.61	3400	274	<5.50	215.5	15	0.066	14.5	1350	5.5	115	5395
CJ-208-105	9.31	1950	330.5	<5.50	581	12.5	0.051	34.5	1200	9.5	105	4229
CJ-209-105	9.77	4650	255	<5.50	371.5	21	0.035	7	2150	5.5	145	7611
CJ-210-105	9.32	1950	355.5	<5.50	478	10	0.047	51	1000	11.5	95	3957
CJ-201-170	9.78	3850	358	<5.50	249	15	0.036	7.5	1825	6	220	6536
CJ-202-170	9.79	4450	225.5	<5.50	269	21.5	0.057	5.5	2050	5	175	7207
CJ-203-170	9.75	3800	345	<5.50	276.5	14	0.054	11	1800	6.5	165	6424
CJ-204-170	9.81	4150	401.5	<5.50	264.5	24	0.062	4.5	1850	5.5	230	6936
CJ-205-170	9.68	4800	301.5	<5.50	274.5	23.5	0.040	3.5	2100	5	235	7749
CJ-206-170	9.76	4600	315.5	<5.50	223.5	22	0.010	5	1950	5	150	7277
CJ-207-170	9.63	3800	289.5	<5.50	276.5	23	0.013	8	1650	5.5	150	6208
CJ-208-170	9.8	5050	302	<5.50	287	19	0.052	4	2200	4.5	165	8037
CJ-209-170	9.51	2950	343.5	<5.50	333.5	18.5	0.033	16.5	1750	6	120	5544
CJ-210-170	9.77	3950	315.5	<5.50	282.5	20.5	0.026	8.5	1800	4.5	115	6502
CJ-201-235	9.81	4100	337.5	<5.50	168	20	0.077	5	1925	5.5	220	6787
CJ-202-235	9.8	4050	306	<5.50	223.5	16.5	0.024	6	1800	5	160	6573
CJ-203-235	9.8	4450	333.5	<5.50	295	25.5	0.031	4	2050	5	240	7409
CJ-204-235	9.74	3250	378	<5.50	301.5	23.5	0.040	9	1600	4.5	165	5737
CJ-205-235	9.67	4500	259.5	<5.50	452	27	0.040	5.5	2200	4.5	130	7584
CJ-206-235	9.71	4200	336.5	<5.50	252.5	26	0.010	6	1850	4.5	145	6826
CJ-207-235	9.75	4550	271	<5.50	269	24	0.013	5.5	2000	4	125	7254
CJ-208-235	9.81	4850	275.5	<5.50	212.5	25.5	0.008	3.5	2100	4	145	7622
CJ-209-235	9.78	4400	303.5	<5.50	297	17	0.043	6.5	1900	4	120	7054
CJ-210-235	9.81	4500	302	<5.50	228.5	19	0.017	5	1950	3.5	115	7129
CJ-201-300	9.86	4650	412	<5.50	180.5	20.5	0.006	4.5	2150	5.5	330	7759
CJ-202-300	9.81	4300	555.5	<5.50	198	16	0.048	8.5	1900	4	540	7528
CJ-203-300	9.7	3800	347.5	<5.50	189	19	0.013	5.5	1800	5	160	6332
CJ-204-300	9.85	4550	270	<5.50	217	22	0.022	1.5	2000	5	160	7231
CJ-205-300	9.73	4250	258.5	<5.50	293.5	23	0.040	6.5	1900	4	125	6866
CJ-206-300	9.63	4300	333	<5.50	103.5	20.5	0.037	6	1850	4.5	125	6748
CJ-207-300	9.76	4700	252	<5.50	292	23	0.007	4	2050	3.5	125	7455
CJ-208-300	9.64	3600	323.5	<5.50	235.5	17.5	0.036	11.5	1550	4	100	5848
CJ-209-300	9.88	5200	252.5	<5.50	172.5	30	0.034	4	2150	4	110	7929
CJ-210-300	9.83	4950	275	<5.50	256	20.5	0.038	4.5	2150	3.5	110	7775
Mean	**9.50**	**3555**	**329**	**<6.21**	**1085**	**18.5**	**0.044**	**189**	**1726**	**29**	**213**	**7151**

pH values in final solution; alkalinity as $CaCO_3$

Estimated Mineralogy of the Crescent Junction Core Samples Based on NETPATH Calculations

Seven elements (C, Ca, Cl, K, Mg, Na, and sulfur [S]) were used to constrain the NETPATH models. After trial and error using a wide range of phase assemblages in NETPATH, seven permissible phases were selected because they produced a reasonable set of results. The selection of permissible phases was aided by XRD (see Section 4.0), and hand-lens observations, and literature on soluble mineral phases that are likely to be present in the Mancos Shale. The minerals selected as permissible phases are calcite, gypsum, thenardite (Na_2SO_4), nahcolite, halite (NaCl), sylvite (KCl), and dolomite [$CaMg(CO_3)_2$]. Cation exchange of Ca and Na was also permitted. Because eight phases (including exchange) were permitted and only seven constraints were used, each sample analysis produced two to three models that exactly match the mass balance constraints. Selection of the model for each sample was somewhat arbitrary, but the major phases are similar among all the models.

The NETPATH results are given in millimole per liter (mmol/L) of test solution (water-soluble extractions). The tests used 2 g of rock in 0.10 L of water. Assuming a porosity of 0.25 and a mineral density of 2500 grams per liter (g/L) for the Mancos Shale at the Crescent Junction Site, a conversion factor of 0.375 is used to convert the NETPATH results to input values for the geochemical modeling program PHREEQC used in Section 8.0 (Parkhurst and Appelo 1999):

$$\frac{0.75\ L_{(rock)}}{0.25\ L_{(gw)}} \times \frac{2500\ g_{(rock)}}{L_{(rock)}} = \frac{7500\ g_{(rock)}}{L_{(gw)}}$$

$$\frac{0.1\ L_{(test\ soln)}}{2\ g_{(rock)}} \times \frac{7500\ g_{(rock)}}{L_{(gw)}} \times \frac{1\ mol_{(mineral)}}{1000\ mmol_{(mineral)}} = \frac{0.375\ mmol_{(mineral)}/L_{(test\ soln)}}{1\ mol_{(mineral)}/L_{(gw)}}$$

where "gw" is ground water and "test soln" is test solution.

The results of the mineral abundances calculated by NETPATH are presented in units of mmol/L of ground water (Table 4). Although thenardite was included in the list of permissible phases, it was not present in any of the selected mineral assemblages (Table 4).

On the basis of the means presented in Table 4, the mineral assemblage is dominated by nahcolite with major amounts of Ca-Na exchange and gypsum. Halite, sylvite, and dolomite occur in lesser amounts. Potassium is contained only in sylvite, thus the concentration of sylvite is constrained by the K concentration. Similarly, the concentration of Mg dictates the concentration of dolomite. All other constraints are contained in more than one phase, and mass balance equations must be solved. Calcite constitutes to 24.23 percent of the soluble mineral mass, but in some simulations calcite had to precipitate to meet the mass balance constraints.

Gypsum and dolomite are more dominant in the samples from the 40-ft depth than in samples from deeper depths (Table 4). Nahcolite and halite are more concentrated in the samples from deeper depths than in the samples from 40-ft depths. Sylvite is concentrated more in the 40-ft and 105-ft samples. The results presented in Table 4 are used in Section 8.3 to designate initial mineral concentrations for a ground water reaction-transport model.

Table 4. Water-Soluble Mineralogy Estimates Based on Mass Balance Approach (expressed as millimole per liter of ground water; negative values indicate precipitation)

Sample	Calcite	Gypsum	Nahcolite	Halite	Sylvite	Ca-Na Exchange	Dolomite
CJ-201-40	–0.07875	0.3075	0.04125	–0.0075	0.09375	0.15375	0.0525
CJ-202-40	0.0075	0.06375	0.20625	–0.0412	0.14625	0.07875	0.01125
CJ-203-40	–1.0125	1.6125	0.975	0.015	0.01875	–0.42	0.12375
CJ-204-40	–0.345	0.6675	0.24375	0.0075	0.01875	0.08625	0.10875
CJ-205-40	0.045	0.06	0.19125	–0.015	0.06375	0.1125	0.0075

Table 4 (continued). Water-Soluble Mineralogy Estimates Based on Mass Balance Approach (expressed as millimole per liter of ground water; negative values indicating precipitation)

Sample	Calcite	Gypsum	Nahcolite	Halite	Sylvite	Ca-Na Exchange	Dolomite
CJ-206-40	–0.0825	0.08625	0.31125	0.03375	0.0225	0.00375	0.01125
CJ-207-40	0.105	0.11625	0.37125	–0.0037	0.045	0.225	0.00375
CJ-208-40	–0.03	0.06375	0.22875	0.0525	0.015	0.03	0.0075
CJ-209-40	–0.1725	0.31875	0.21	–0.0112	0.0375	0.15375	0.05625
CJ-210-40	0.05625	0.06	0.36375	0.0225	0.03	0.11625	0.00375
CJ-201-105	0.0525	0.03	0.195	0.045	0.02625	0.075	0.00375
CJ-202-105	0.0675	0.015	0.40125	0.01875	0.165	0.0825	0.00375
CJ-203-105	0.09	0.03	0.21	0.03	0.1575	0.11625	0.00375
CJ-204-105	0.135	0.01875	0.34125	0.00375	0.0525	0.15375	0.00375
CJ-205-105	0.045	0.02625	0.49125	0.03375	0.045	0.07125	0.00375
CJ-206-105	–0.015	0.03375	0.28125	0.045	0.0225	0.0225	0.01125
CJ-207-105	–0.0375	0.015	0.44625	0.0375	0.0225	–0.01875	0.00375
CJ-208-105	0.0075	0.045	0.24	0.04875	0.01875	0.04875	0.00375
CJ-209-105	0.08625	0.03	0.43875	0.02625	0.02625	0.11625	0.00375
CJ-210-105	–0.04125	0.0375	0.28875	0.05625	0.01875	–0.01125	0.00375
CJ-201-170	0.09	0.01875	0.345	0.03375	0.04125	0.10875	0.00375
CJ-202-170	0.1125	0.0225	0.39	0.015	0.03375	0.13125	0.00375
CJ-203-170	0.07125	0.0225	0.36375	0.04125	0.03	0.09	0.00375
CJ-204-170	0.06	0.0225	0.40125	0.04125	0.045	0.0825	0.00375
CJ-205-170	0.0525	0.0225	0.51375	0.01875	0.045	0.07875	0.00375
CJ-206-170	0.0375	0.01875	0.4875	0.0375	0.03	0.05625	0.00375
CJ-207-170	0.0075	0.0225	0.44625	0.03375	0.03	0.03	0.00375
CJ-208-170	0.0675	0.0225	0.49875	0.03375	0.03	0.09375	0.00375
CJ-209-170	0.105	0.02625	0.255	0.04875	0.0225	0.13125	0.00375
CJ-210-170	0.0525	0.0225	0.39375	0.045	0.0225	0.075	0.00375
CJ-201-235	0.11625	0.01125	0.34125	0.03	0.04125	0.13125	0.00375
CJ-202-235	0.06375	0.01875	0.39	0.03375	0.03	0.0825	0.00375
CJ-203-235	0.10125	0.0225	0.3975	0.0225	0.045	0.12375	0.00375
CJ-204-235	0.06	0.0225	0.3075	0.04875	0.03	0.0825	0.00375
CJ-205-235	0.08625	0.03375	0.44625	0.03	0.02625	0.12	0.00375
CJ-206-235	0.03375	0.01875	0.45375	0.045	0.02625	0.0525	0.00375
CJ-207-235	0.0525	0.0225	0.465	0.03375	0.0225	0.075	0.00375
CJ-208-235	0.07875	0.015	0.465	0.03	0.02625	0.09375	0.00375
CJ-209-235	0.03375	0.0225	0.465	0.04125	0.0225	0.05625	0.00375
CJ-210-235	0.05625	0.01875	0.45	0.04125	0.0225	0.07125	0.00375
CJ-201-300	0.13875	0.015	0.3675	0.0225	0.06375	0.15375	0.00375
CJ-202-300	0.09375	0.015	0.38625	0.015	0.105	0.10875	0.00375
CJ-203-300	0.07125	0.015	0.3675	0.04125	0.03	0.08625	0.00375
CJ-204-300	0.09	0.01875	0.40875	0.02625	0.03	0.10875	0.00375
CJ-205-300	0.0525	0.0225	0.43875	0.03	0.0225	0.075	0.00375
CJ-206-300	0.0225	0.0075	0.495	0.045	0.0225	0.03	0.00375
CJ-207-300	0.05625	0.0225	0.48375	0.03	0.0225	0.07875	0.00375
CJ-208-300	–0.0075	0.01875	0.435	0.04875	0.01875	0.01125	0.00375
CJ-209-300	0.07875	0.015	0.4875	0.03375	0.0225	0.09	0.00375
CJ-210-300	0.17625	0.01875	0.27	0.0375	0.0225	0.19875	0.00375
Mean	**0.0199**	**0.0847**	**0.3779**	**0.0287**	**0.0406**	**0.0781**	**0.0109**

3.0 Cation Exchange Capacity

3.1 Introduction

CEC is the ability of a solid substance to freely exchange one cation for another. For example, cations in smectite clay minerals are able to readily enter and exit the interlayer (exchangeable) sites. Cations are selective in their ability to occupy exchange sites, and selectivity is often influenced by the hydration state of the dissolved cation. CEC can be dependent on other solution variables such as pH values. CEC is commonly expressed in units of milliequivalents per 100 grams (meq/100 g). Typical values of CEC for pure clays are 3 to 15 meq/100 g for kaolinite, 80 to 150 meq/100 g for smectite, and 10 to 40 meq/100 g for illite (Grim 1953). Mancos Shale samples analyzed in this study contain mostly kaolinite, illite, and smectitic interlayered clay minerals (Section 4.0).

Because clay minerals are abundant, the Mancos Shale may have a large CEC that can cause significant changes to ground water chemistry. Knowledge of the CEC is required to develop a geochemical model of water–rock interactions. It is assumed that most of the CEC in the Crescent Junction samples is due to the clay minerals. In the reaction-transport modeling, presented in Section 8.5, the CEC is considered a fixed property of the rock, but selectivity of cations occupying the exchange sites is controlled by solution chemistry. The laboratory results presented in this section are used to specify the number of exchange sites in the models.

3.2 Methods

CEC was measured on 20 core samples of Mancos Shale collected from 40-ft and 105-ft depths. Samples were crushed, air dried, and sieved to –10 +18 mesh (1- to 2-mm nominal diameter) in the same manner as for the other tests. This size fraction was selected because it is easy to work with in small-scale CEC tests and has a reasonably constant surface area (Section 5.0). The results could be scaled to field conditions by normalizing to the surface area. CEC was also measured on a powdered Mancos Shale sample to provide information on maximum CEC.

Various methods have been used to measure CEC. Most methods rely on saturation of the exchange sites with a single composition of cation; subsequently the cation is removed from the fully saturated mineral and its mass is measured to determine CEC. No general method exists that can be reliably used for all clay-bearing samples (Bain and Smith 1987). Methods include saturation with barium (Ba), Ca, K, Na, or NH_4, (Jackson 1969; Bain and Smith 1987).

In this study, CEC was determined using the ammonium saturation method (Chapman 1965 as described in Bain and Smith 1987). This method was selected largely because the saturating solution (ammonium acetate) is highly buffered and maintains its near-neutral pH value throughout the test (Chapman 1965). Another advantage is that NH_4 concentrations are easily measured in the sodium-chloride extracts. Accuracy of the method was checked by measuring the CEC of a calcium-montmorillonite clay standard (sample number STx-1) from the Source Clay collection of the Clay Minerals Society. CEC values published by Borden and Giese (2001) for this specimen were 89 meq/100 g with a standard deviation of 2 meq/100 g. CEC values of nine repetitions in our laboratory ranged from 71.4 to 85.7 meq/100 g with a mean of 77.0 and a standard deviation of 6.6. Although slightly lower than the Borden and Giese (2001) results, our values are reasonably similar and probably within the range of analytical uncertainty.

For the ammonium saturation method, the clay sample was first saturated with NH_4 ions using 1 molar (M) ammonium acetate followed by exchange with sodium chloride (STO 210, method CB [CEC-1]). For a CEC measurement, an exact weight of clay ranging from 20 milligrams (mg) to 200 mg was combined with 20 mL of 1 M ammonium acetate and agitated end over end for 2 hours. The solids were separated from the liquid phase by centrifugation, and the saturation process with ammonium acetate was repeated five times. Isopropyl alcohol (20 mL) was then added to the solids, the mixture was agitated by hand, and centrifuged. Five additional washings with isopropyl alcohol were conducted, after which 20 mL of 100 g/L sodium chloride solution was added to the solid phases to initiate removal of the NH_4 cations from the exchange sites. The sodium chloride solution was agitated by hand seven times. The NH_4 concentration in the resultant solution was measured spectrophotometrically and was used to calculate the CEC.

3.3 Results and Discussion

CEC measurements ranged from 0.54 to 36.29 meq/100 g with a mean of 11.23 meq/100 g (Table 5). The mean is within the range published by Grim (1953) for pure kaolinite (3 to 15 meq/100 g) and pure illite (10 to 40 meq/100 g) but is significantly less than pure smectite (80 to 150 meq/100 g). The values for these Mancos Shale samples are reasonable for the clay mineral compositions as determined by XRD analysis (Section 4.0).

One sample (CJ-205-40) was ground to a powder to compare CEC values for a finer grain size. The CEC measurements of the powder (10.29 and 10.43 meq/100 g for duplicate samples) were similar to the 1- to 2-mm grain size. Although limited to one analysis, this result provides confidence for applying the laboratory CEC values to the field in the reaction-transport models (Section 8.5). The CECs are used in the reaction-transport models to simulate cation exchange of Ca, K, NH_4, and Na. Retardation of NH_4 in the model is assumed to be caused by the cation exchange with the Mancos Shale.

Table 5. Results of Cation Exchange Measurements

Sample ID[a]	Size Fraction	CEC (meq/100 g)
CJ-201-40	1 to 2 mm	9.29
CJ-202-40	1 to 2 mm	11.71
CJ-203-40	1 to 2 mm	36.29
CJ-204-40	1 to 2 mm	10.71
CJ-205-40	1 to 2 mm	10.71
CJ-205-40-Dup	1 to 2 mm	12.71
CJ-205-40-P	<1 mm	10.29
CJ-205-40-P-Dup	<1 mm	10.43
CJ-206-40	1 to 2 mm	5.86
CJ-207-40	1 to 2 mm	15.43
CJ-208-40	1 to 2 mm	7.00
CJ-209-40	1 to 2 mm	17.00
CJ-210-40	1 to 2 mm	11.43
CJ-201-105	1 to 2 mm	5.29
CJ-202-105	1 to 2 mm	11.43
CJ-203-105	1 to 2 mm	7.00
CJ-204-105	1 to 2 mm	12.86
CJ-204-105-Dup	1 to 2 mm	13.14
CJ-205-105	1 to 2 mm	12.43
CJ-206-105	1 to 2 mm	7.43
CJ-207-105	1 to 2 mm	8.57
CJ-208-105	1 to 2 mm	7.14
CJ-209-105	1 to 2 mm	14.71
CJ-210-104	1 to 2 mm	0.54
Minimum		0.54
Maximum		36.29
Mean		11.23

[a]P = Powdered Sample, Dup = Duplicate

A brief literature search was conducted to determine if the CEC values of Crescent Junction Mancos Shale samples are comparable to CEC measurements of Mancos Shale samples from other areas. Evangelou et al. (1984) collected samples of partially weathered and unweathered outcrop samples of Mancos Shale from the West Salt Creek watershed near Grand Junction, Colorado, and analyzed the CEC using the calcium/barium exchange method. They reported CEC values ranging from 13.25 to 19.96 meq/100 g. These values are similar to the Crescent Junction values and suggest that the CEC for Mancos Shale may be relatively constant.

4.0 X-Ray Diffraction Analysis

4.1 Introduction

XRD was used to identify minerals present in the core samples. XRD is capable of defining the internal arrangement of atoms in a crystalline lattice, thus making it possible to positively identify minerals. Identification of mineralogy based on chemical methods (Section 2.3.2) is more ambiguous because often minerals have similar chemical compositions and, in some cases, identical compositions. Unlike chemical methods, XRD analysis is not able to detect small quantities of minerals (XRD is generally limited to detection of approximately 10 percent, but detection is dependent on mineral crystallinity) and only semi-quantitative estimates of mineral abundances are possible. XRD analyses were conducted at Mesa State College in Grand Junction, Colorado, by Dr. William Hood (Appendix D).

Chemical interaction between ground water and Mancos Shale is likely to occur mostly at the surfaces of clay minerals. Therefore, clay mineral chemistry is important to the transport of contaminants by the ground water. XRD is one of the best analytical tools to identify clay minerals. For this study, 10 core samples, all from the 40-ft depth, were analyzed by XRD.

For XRD analysis, the sample is subjected to an x-ray beam. The atomic lattice within the individual mineral crystals diffracts (reflects) the x-ray beam, and the angle of diffraction is measured. The angle of diffraction and the intensity of the diffracted x-rays produce a “fingerprint” that can be used to identify the minerals (Jackson 1969).

4.2 Methods

A random powder mount was used for identification of major minerals (Appendix D). Samples were finely powdered with a mortar and pestle, and placed in a sample holder, and scanned from 4.2 to 50 degrees 2θ using a Rigaku Miniflex x-ray diffractometer (Appendix D). The Jade computer program was used to calculate spacings and to compare diffraction patterns of the samples with diffraction patterns of known minerals.

Splits of the samples were analyzed for clay mineralogy (Appendix D). Analysis of clay mineralogy is more complex than for the major minerals because the sample requires four separate preparation methods and an XRD analysis of each. To prepare the clay mineral splits, the clays were segregated into fine particles and not flocculated. The bulk sample was first placed in water overnight to remove readily soluble material and initiate disaggregation of the clays. Calgon (sodium metaphosphate) was added to further disperse clay minerals and the mixture was allowed to sit for 8 hours. Magnesium was added to the suspension to saturate the clay mineral interlayers (to produce a constant d spacing of this lattice plane). A small quantity of the suspension was smeared on a glass microscope slide and allowed to dry. The four methods used to treat the clay mineral separates are (1) air drying, (2) glycolating, (3) heating to 300 ºC, and (4) heating to 550 ºC. More details on the preparation and analysis methods are available in Appendix D. XRD patterns from these four treatments were used to positively identify the clay minerals and to estimate the amount of smectite layers in interlayered illite/smectite clays.

Estimates of the mineral abundance of non-phyllosilicate minerals were made by a process including background removal, normalizing the peak intensities to a quartz standard, and summing the peak intensities. Estimates of clay mineral abundance used the glycolated diffractograms and employed a series of computer enhancements, including background removal and peak assessment. The ratio of illite to smectite layers in the mixed-layer clays was estimated from a comparison of the Mg-saturated and glycolated diffractograms. More details on the methods used to estimate mineral abundances are

presented in Appendix D. X-ray diffraction methods provide only a semi-quantitative estimate of the mineral abundances. According to Schultz (1964) based on his work with Pierre Shale (a Mancos Shale equivalent), the abundance estimates are adversely affected by sampling, sample preparation, machine response, and, most importantly, interpretation. Schultz (1964) also states that if a mineral makes up more than 15 percent of the sample, the precision of the abundance estimate is usually within about 10 percent. At lower mineral concentrations, the uncertainty increases.

4.3 Results and Discussion

XRD analysis was conducted on the 10 samples of Mancos Shale collected from the 40-ft depth. The mineralogical composition of these samples is dominated by quartz, with lesser amounts of dolomite and calcite, small amounts of feldspar, and traces of gypsum (Table 6.). Orthoclase and plagioclase feldspar occur in approximately equal amounts.

Table 6. Non-Phyllosilicate Mineral Abundance Estimates in Percent Based on XRD Analysis of Bulk Samples

Sample ID	Quartz	Calcite	Dolomite	Orthoclase	Plagioclase	Gypsum
CJ-201-40	32	3	5	1	1	Tr[a]
CJ-202-40	29	3	4	1	1	1
CJ-203-40	36	4	5	1	2	1
CJ-204-40	33	2	3	1	1	
CJ-205-40	28	3	6	1	1	
CJ-206-40	39	4	6	1	2	
CJ-207-40	25	3	3	1	1	
CJ-208-40	38	3	5	1	1	
CJ-209-40	27	1	3	2	1	Tr
CJ-210-40	24	4	3	1	1	

[a]Tr = trace.

The clay mineral fraction is dominated by mixed-layer (mostly illite/smectite) clays, illite, and kaolinite (Table 7.). The mixed-layer clays are dominated by illite layers. A small amount of mixed-layer chlorite/vermiculite is probably present.

Table 7. Estimates of Clay Mineral Abundance in Percent of Total Clay Based on XRD Analysis

Sample ID	Mixed Layer[a]	Illite	Kaolinite	Percent Illite in Mixed-Layer Clays
CJ-201-40	43	29	28	70
CJ-202-40	38	36	26	60
CJ-203-40	43	31	25	60
CJ-204-40	40	30	29	60
CJ-205-40	46	31	23	60
CJ-206-40	37	34	29	60
CJ-207-40	27	36	37	50
CJ-208-40	35	36	29	60
CJ-209-40	39	31	29	60
CJ-210-40	39	37	25	60

[a]Mostly mixed-layer illite/smectite with minor chlorite/vermiculite.

A brief literature survey was conducted to determine if the XRD results for the Mancos Shale at Crescent Junction are typical of other Mancos Shale localities. Schultz (1997) reported that clays in the Mancos Shale from the Colorado Plateau region contain 50 to 60 percent mixed-layer illite/smectite, 12 to 15 percent poorly ordered kaolinite, and 30 to 35 percent illite; however, no source of data is provided in that publication. Nadeau and Reynolds (1981b) discuss clay mineral XRD results of 77 bentonite-shale paired samples collected from the Mancos Shale throughout the western interior of North America. They determined that the clays are primarily randomly mixed-layer illite/smectite with illite compositions ranging from 0 to 85 percent. They attribute the origin of the clays to volcanic ash. The illitic component increases in response to increased burial metamorphism, as does the ordering of the illite/smectite.

Nadeau and Reynolds (1981a) discuss XRD clay mineralogy results of 690 samples of Mancos Shale collected from 154 sites in the four-state region of Colorado, Utah, Arizona, and New Mexico. These clays are dominated by mixed-layer illite/smectite, with 20 to 60 percent illite layers. The regional distribution of ordering in the mixed-layer illite/smectite is attributed to differences in burial metamorphism of the Mancos Shale. Evangelou et al. (1984) collected samples of partially weathered and unweathered outcrop samples of Mancos Shale from the West Salt Creek Watershed near Grand Junction, Colorado, and analyzed the clay fractions by XRD. These clay fractions contain mica, kaolin, smectite, and randomly interstratified mixed-layer clay, possibly mica/vermiculite. These studies generally indicate that the clays identified in the Crescent Junction samples (kaolinite, illite, and mixed-layer illite/smectite) are typical of the Mancos Shale throughout much of its depositional basin.

5.0 Surface Area

5.1 Introduction

Knowledge of the surface area of the Mancos Shale samples is needed to relate the results to the transport of contaminants through the subsurface. Processes such as cation exchange and adsorption are directly related to the surface area that the ground water contacts. For example, for the same travel distance, interaction of dissolved contaminants with the rock will be less in a fracture-dominated matrix (small surface area) than in a porous-media (higher surface area) flow. It is beyond the scope of this study to determine the nature of the flow (fracture versus porous media) in the subsurface at the Crescent Junction Site. However, to properly use the data collected during this study in site models, these data will need to be normalized to surface area. Therefore, it is important to measure the surface area of the samples used in the tests. Surface area was determined for 10 core samples from the 40-ft depth.

5.2 Methods

Samples were crushed, air dried, and sieved to –10 +18 mesh (1- to 2-mm nominal diameter) in the same manner as for other tests. Surface area was determined by the standard BET method. This method is the most widely used method for determining particle surface area. Samples were prepared by heating while simultaneously evacuating to remove impurities. The prepared samples were then cooled with liquid nitrogen and analyzed by measuring the volume of N_2 gas adsorbed at specific pressures (Micromeritics 2006; Jackson 1969). Multiple-point isotherm measurements were conducted. The multiple point tests are more accurate than single point tests. Micromeritics Analytical Services (2006), Norcross, Georgia, conducted the surface area measurements (Appendix E).

5.3 Results and Discussion

Measured surface areas of the 10 samples from the 40-ft depth range from 8.81 to 13.22 square meters per gram (m^2/g) with a mean of 11.02 m^2/g (Table 8.). These values are reasonably comparable to surface areas measured by Davis and Curtis (2003) on alluvial aquifer samples obtained from the former Naturita, Colorado, uranium-ore processing site. Surface areas measured on the 16 Naturita samples range from 5.2 to 20.0 m^2/g with a mean of 12.43 m^2/g and standard deviation of 3.77 m^2/g. Surface area was used as an input to the surface-complexation algorithm in the transport model presented in Section 8.4.

Surface area was also measured on a powdered split of Crescent Junction sample CJ-205-40. The surface area of the powdered sample (10.7 m^2/g) is consistent with surface areas measured on the 1- to 2-mm fractions, indicating that the BET method is probably accounting for intraparticle surface area.

Table 8. Results of BET Surface Area Analysis of 1- to 2-mm Size Fraction

Sample ID	Surface Area (m^2/g)
CJ-201-40	10.65
CJ-202-40	12.21
CJ-203-40	8.81
CJ-204-40	12.92
CJ-205-40	9.95
CJ-206-40	9.46
CJ-207-40	13.12
CJ-208-40	9.39
CJ-209-40	10.46
CJ-210-40	13.22
Minimum	8.81
Maximum	13.22
Mean	11.02

6.0 Distribution Ratios

6.1 Introduction

Distribution ratios (R_d) are a measure of the partitioning of a contaminant between the ground water and the solid fraction of the aquifer. The higher the R_d value, the more partitioning to the solids and the more retardation of the contaminant. The R_d value is empirical and is simply the ratio of the measured concentration in the solids (milligrams per kilogram [mg/kg]) to the measured concentration in the ground water (milligrams per liter [mg/L]), and has units of milliliters per gram (mL/g). R_d values are often used to simulate retardation of contaminants in ground water models. When used in these models, an implicit assumption exists that chemical retardation occurs by the process of adsorption under equilibrium conditions. For the equilibrium assumption, the R_d value is often referred to as a distribution coefficient (K_d). Many models also assume that K_d does not vary with the concentration of the contaminant, but research has shown that it often does, and algorithms such as the Langmuir or Freudlich equations are used to produce a better fit to R_d data. To test if R_d values vary with contaminant concentrations, multiple points using various concentrations are measured, and plots of these “adsorption isotherms” are fitted with the various models. If the plot is reasonably linear, then models using a constant K_d value (also termed linear isotherm) will produce satisfactory results.

The R_d value can vary significantly with solution chemistry. For example, Davis et al. (2004) show that R_d values for U in a sample of alluvium vary by more than a factor of 10, depending on dissolved carbonate concentrations and pH values. Also, the R_d approach is only valid for contaminants that occur in trace concentrations.

For the reaction-transport modeling, a surface-complexation approach is employed instead of using R_d values to simulate retardation of U (Section 8.4). With the surface-complexation approach, the R_d value changes as chemical conditions (especially pH and pCO_2) change in the aquifer. The main use of the R_d values determined in this study is to test and calibrate the surface-complexation module used in the reaction-transport modeling.

6.2 Methods

Uranium R_d values were determined using procedure CB (Rd-1) in STO 210. In summary, a sample of Mancos Shale was crushed and sieved to –10 +18 mesh (1- to 2-mm nominal diameter). The sample (5 g for a single-point R_d value) was placed in a plastic centrifuge tube with 100 mL of pH value-adjusted synthetic pore fluid (SPF) that simulates tailings or evolved pore fluid. The tubes were agitated end over end for 24 hours and then centrifuged, decanted, and filtered through a 0.45-micrometer (µm) filter. Filtrates were analyzed for electrical conductivity, pH value, alkalinity, and U concentration. Controls included SPF without solids and duplicates. The concentration of U in the solid phase was determined from the loss of U from the SPF solution. R_d values were determined from the calculated concentration of U in the solid phase and the measured U concentration in the solution.

Uranium R_d values were determined using three different SPF compositions designed to simulate ground water that could be present in the Mancos Shale after construction of the disposal cell. One solution (SPF-1) simulates pore fluids that currently exist in the tailings. Another solution (SPF-2) simulates tailings pore water mixed with 50 percent Mancos Shale ground water. A third solution (SPF-3) simulates water that results from the sequential batch-leaching testing (Section 7.0). Table 9 provides compositions of the SPF fluids. The SPF solutions were spiked with 1 mg/L U to enable measurement of the R_d values.

Table 9. Composition (milligrams per liter) of SPF Used in Uranium R_d Tests

Constituent	SPF-1	SPF-2	SPF-3
Sodium	5,781.41	5,888.61	7,806.64
Potassium	112.23	76.31	166.10
Calcium	209.62	148.48	195.65
Magnesium	315.71	197.32	179.56
Ammonium	2,181.82	1,036.36	900.00
Sulfate	17,454.37	14,606.17	17,913.58
Chloride	910.26	[a]309.49	1,365.38
Inorganic Carbon	271.43	314.29	78.57
pH Value	6.63	6.96	7.97

[a]The value for Cl for SPF-2 should have been approximately 4,541 mg/L. The low value (309.49) resulted from an error in designing the SPF-2 solution.

Single-point R_d measurements for U were determined for 20 samples, and 6-point isotherms were determined for five samples of SPF-1. For the five samples used for isotherms, single-point R_d values were also determined using SPF-2 and SPF-3 to evaluate sensitivity to solution chemistry.

6.3 Results and Discussion

R_d values were corrected for the amount of “labile” U contained in the Mancos Shale samples. The labile U fraction is defined as U in the solid fraction capable of being released to the solution during a test (Davis et al. 2004). Release of labile U is usually a function of time with longer agitation periods resulting in higher concentrations of labile U. A constant value of 0.0436 µg/g for the labile U fraction was used in our study. This value is the mean of eight measurements of the sequential batch-leaching tests (Section 7.0). In the sequential batch tests, U-free SPF was reacted for various time periods with Mancos Shale samples, and U concentrations were measured in the final solutions. For comparison, Davis et al. (2004) used a value of 0.21 µg/g for labile U in uncontaminated alluvial aquifer sediment from the Naturita Site.

Despite making corrections for the labile U, some tests produced negative R_d values (Table 11). Negative R_d values are a combination of (1) analytical uncertainty, (2) relatively low R_d values, and (3) variable contribution from labile U. Minimum and maximum R_d values presented in the tables in this section are based on analytical imprecision of ±2.5 percent in all U measurements. Many of the R_d determinations were fairly sensitive to the analytical imprecision.

Single-point determinations of R_d using SPF-1 (tailings fluid) ranged from negative values to 0.84 mL/g (Table 10). The maximum R_d value, accounting for 2.5 percent error in all measurements, is 1.9 mL/g. These values are reasonably similar to R_d values measured on alluvial aquifer material from other uranium-ore milling sites. For example, R_d values for samples collected at the DOE New Rifle, Colorado, Site, for alluvium and Wasatch Formation, range from negative values to 3.7 mL/g and 1.6 mL/g, respectively (DOE 1999).

Table 10. Final Concentrations of U in Liquid (U_l) and Solid (U_s) Phases and R_d for Single-Point Determination with SPF-1[a]

Sample ID	U_l (µg/L) Measured	U_s (µg/g) Calculated	R_d (mL/g)	R_d (mL/g) Minimum	R_d (mL/g) Maximum
CJ-201-40	898.0	–1.33	–1.48	–2.38	–0.53
CJ-202-40	805.4	0.28	0.34	–0.65	1.39
CJ-203-40	892.2	–1.21	–1.36	–2.27	–0.40
CJ-204-40	890.9	–1.19	–1.33	–2.24	–0.38
CJ-205-40	793.9	0.51	0.64	–0.37	1.70
CJ-206-40	906.1	–1.49	–1.64	–2.54	–0.70
CJ-207-40	811.6	0.15	0.19	–0.79	1.22
CJ-208-40	753.6	0.54	0.72	–0.29	1.78
CJ-209-40	926.6	–1.90	–2.05	–2.93	–1.13
CJ-210-40	757.6	0.46	0.61	–0.39	1.67
CJ-201-105	850.1	–0.37	–0.44	–1.39	0.57
CJ-202-105	839.4	–0.16	–0.19	–1.15	0.83
CJ-203-105	821.2	0.21	0.25	–0.73	1.29
CJ-204-105	822.4	0.18	0.22	–0.76	1.26
CJ-205-105	839.3	–0.15	–0.18	–1.15	0.83
CJ-206-105	852.1	–0.41	–0.48	–1.43	0.52
CJ-207-105	798	0.67	0.84	–0.17	1.91
CJ-208-105	805.6	0.52	0.64	–0.36	1.70
CJ-209-105	813.6	0.36	0.44	–0.55	1.49
CJ-210-105	819.4	0.24	0.30	–0.69	1.34
SPF-1	829.4				

[a]Test conditions: pH 7.57, alkalinity 570 mg/L $CaCO_3$, 50 g/L. Minimum and maximum R_d values based on ±2.5 percent for U analyses on final solutions and SPF-1.

Single-point R_d values for samples from the 40-ft depth using SPF-2 (simulated tailings pore water mixed with 50 percent Mancos Shale ground water) range from –0.46 to 0.51 mL/g with one negative value (Table 11). Single-point R_d values for samples from the 40-ft depth using SPF-3 (simulated water that results from the sequential batch-leaching testing) ranged from 0.41 to 1.92 mL/g (Table 12). Maximum R_d values for SPF-2 and SPF-3 are 1.56 and 3.04 mL/g, respectively. The R_d values for SPF-3 are slightly higher than those of the SPF-1 and SPF-2 solutions, indicating increased partitioning to the solid phase. This might be expected for SPF-3, as it has a much lower dissolved carbon concentration and a higher pH value (Table 9).

Table 11. Final Concentrations of U in Liquid (U_l) and Solid (U_s) Phases and R_d for Single-Point Determination with SPF-2[a]

Sample ID	U_l (µg/L) Measured	U_s (µg/g) Calculated	R_d (mL/g)	R_d (mL/g) Minimum	R_d (mL/g) Maximum
CJ-202-40	760.4	0.22	0.29	–0.70	1.33
CJ-205-40	765.0	0.13	0.17	–0.82	1.20
CJ-207-40	756.1	0.31	0.40	–0.59	1.45
CJ-208-40	789.5	–0.36	–0.46	–1.41	0.54
CJ-208-40D	752.1	0.39	0.51	–0.49	1.56
CJ-210-40	761.0	0.21	0.27	–0.71	1.31
SPF-2	769.2				

[a]Test conditions: pH 7.69, alkalinity 907 mg/L $CaCO_3$, 50 g/L. Minimum and maximum R_d values are based on ±2.5 percent for U analyses on final solutions and SPF-2. D in sample ID number indicates duplicate analysis.

Table 12. Final Concentrations of U in Liquid (U_l) and Solid (U_s) Phases and R_d for Single-Point Determination with SPF-3[a]

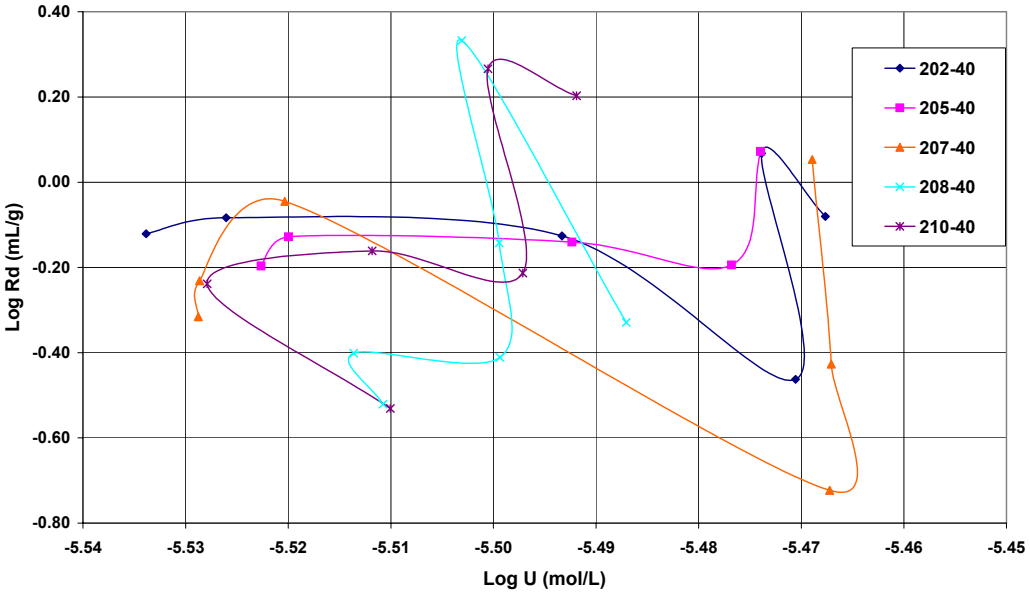
Sample ID	U_l (µg/L) Measured	U_s (µg/g) Calculated	R_d (mL/g)	R_d (mL/g) Minimum	R_d (mL/g) Maximum
CJ-202-40	742.2	1.42	1.92	0.85	3.04
CJ-205-40	756.7	1.13	1.50	0.45	2.60
CJ-207-40	783.4	0.60	0.77	–0.25	1.83
CJ-208-40	797.0	0.33	0.41	–0.58	1.46
CJ-210-40	793.9	0.39	0.49	–0.51	1.54
SPF-3	811.2				

[a]Test conditions: pH 7.91, alkalinity 313 mg/L $CaCO_3$, 50 g/L. Minimum and maximum R_d values are based on ±2.5 percent for U analyses on final solutions and SPF-3.

Isotherm tests using mass-to-water ratios of 10, 20, 50, 100, 200, and 250 g/L were conducted on five Mancos Shale samples from the 40-ft depth using SPF-1. For a linear isotherm, the results should plot as a straight line on a log-log plot such as shown on Figure 1a. The lack of linearity of these plots is likely due in large part to analytical imprecision. The analytical uncertainty is greatest at the highest values of dissolved U (Figure 1b). Better definition would result if the tests had spanned a larger range of U concentrations and used larger masses of solids. Although these data are scattered, it is apparent that the uranium R_d values of the Crescent Junction Mancos Shale samples are relatively low.

The same data shown on Figure 1a are plotted on Figure 2 at a larger scale, along with the Naturita uranium R_d results from Davis et al. (2004). Data from Crescent Junction form a relatively tight group near the dissolved U concentration of $10^{-5.50}$ mol/L. Many of the Crescent Junction sample uranium R_d values are lower than any of the Naturita results. The lowest Naturita R_d values were measured on solutions with high CO_2 partial pressures and a near-neutral pH value of 6.88 (Davis1 on Figure 2). The Crescent Junction SPFs also have high CO_2 concentrations and near-neutral pH (Table 9), which accounts for their low R_d values. The mineralogy of the Mancos Shale (e.g., low in iron oxyhydroxide) compared to alluvial samples may also be partly responsible for the lower R_d values.

a.



b.

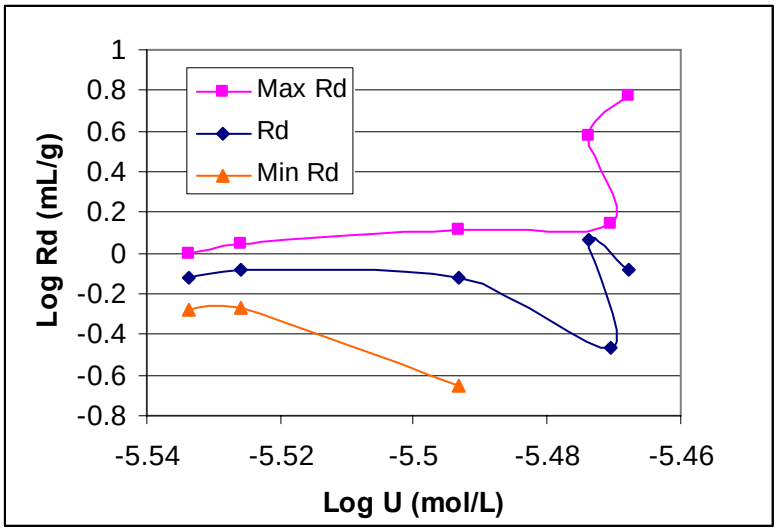
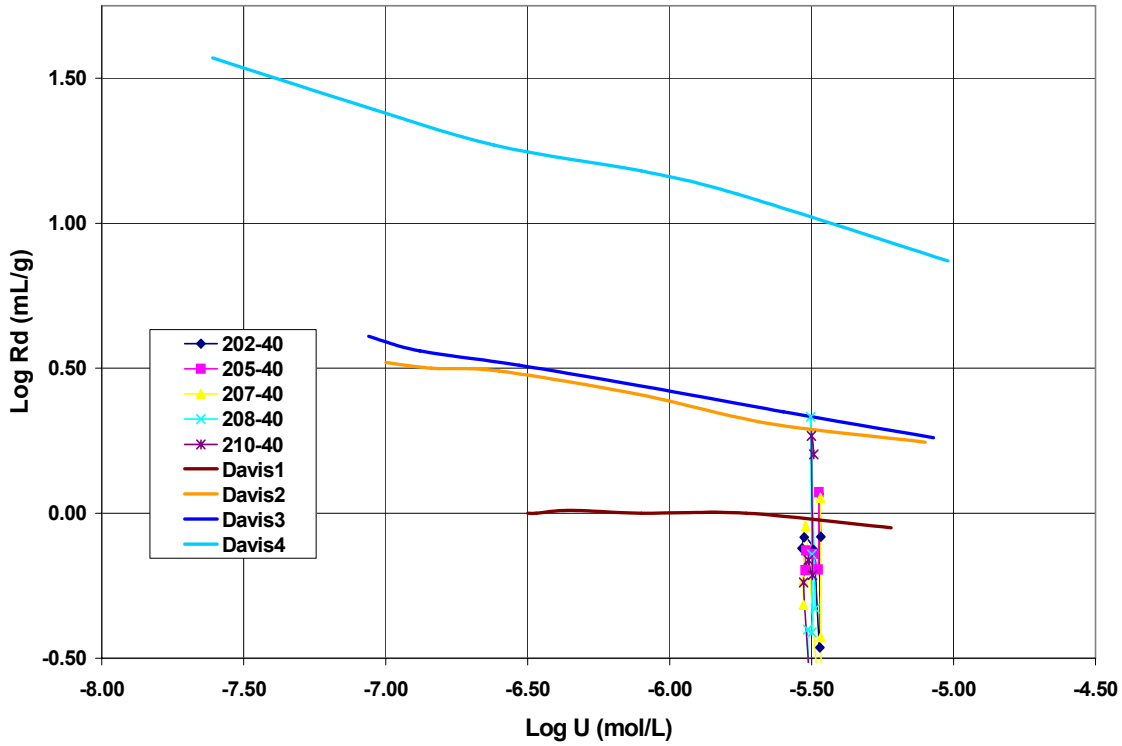


Figure 1. a. Isotherm Plot of Uranium R_d Determinations Made on Crescent Junction Mancos Shale Sample Using SPF-1

b. Isotherm Plot of Sample 202-40 Showing Effect of Analytical Imprecision on Calculated Uranium R_d Values; Maximum and Minimum R_d Values are Calculated Using $\pm$2.5% Uncertainty on all Analytical Measurements.



Davis1 = AGW-6, pH 6.88, 6.8 percent CO_2, 820 g/L
Davis2 = AGW-5, pH 7.18, 1.57 percent CO_2, 250 g/L
Davis3 = AGW-7, pH 7.58, 0.47 percent CO_2, 125 g/L
Davis4 = AGW-3 (laboratory air), pH 7.94, 0.05 percent CO_2, 25 g/L

Figure 2. Comparison of Uranium R_d Determinations Made on Crescent Junction Mancos Shale Samples Using SPF-1 to Data from the Naturita Site by Davis et al. (2004)

The uranium R_d values from our testing are more scattered than the results measured by Davis et al. (2004) on the Naturita samples. The scatter is largely due to the lower rock-to-water ratios used in our tests. Davis et al. (2004) used up to 820 g/L, whereas, we used a maximum of 250 g/L. Because of the low R_d values, a higher rock-to-water ratio would have reduced the scatter in our data. However, we believe that additional measurements at higher rock-to-water ratios are unnecessary because the results are not likely to change the conclusion that the parameters used in the Davis et al. (2004) model are a reasonable approximation for use at the Crescent Junction Site.

7.0 Sequential Batch-Leaching Tests

7.1 Introduction

Two sequential batch-leaching tests were conducted to measure evolution of tailings leachate chemistry as it interacts with Mancos Shale. Results of these tests were used to help calibrate the reaction transport models presented in Section 8.7. In the sequential batch-leaching tests, the test fluid (SPF-1) was not spiked with U as it was for the R_d tests (Section 6.2). Rather, any U in the solution was released from the Mancos Shale samples. The evolution of major-ion chemistry and pH were monitored to determine the effects of these changes on U partitioning.

7.2 Methods

A 100-g sample of Mancos Shale was crushed, air dried, and sieved to –10 +18 mesh (1- to 2-mm nominal diameter). The sample was combined with 400 mL of SPF-1 in a 500-mL glass Erlenmeyer flask, agitated on an orbital shake table for 24 hours, and then centrifugated, decanted, and filtered (0.45 µm) to separate solids from the solution. A 50-mL split was retained and analyzed for pH, ORP, specific conductance, alkalinity, Ca, Cl, K, Mg, Na, NH_3, NO_3, SO_4, and U. The remaining solution was placed with approximately 87.5 g of the next Mancos Shale sample. The exact amount of the Mancos Shale sample was calculated so that the water-to-rock ratio remained constant. The procedure was repeated to monitor the changing solution composition as the fluid reacted with progressively more Mancos Shale.

7.3 Results and Discussion

Two sequential batch-leaching tests were conducted, one to simulate vertical transport and one to simulate horizontal transport through the Mancos Shale. To simulate horizontal transport, the 40-ft-depth samples from borings CJ-203, -204, and -206 were used, in that order. Chemical changes that occurred in the solution as it reacted with progressively more Mancos Shale include slightly increasing values of pH, Cl, K, Na, SO_4, and U. Small decreases occurred in ORP and NH_3-N, while alkalinity, Ca, and Mg remained fairly stable (Table 13). The increase in U may be caused by longer reaction times with the sediment or by decreasing R_d values because of increasing pH values and nearly constant dissolved carbonate concentration.

To simulate vertical transport, SPF-1 (Table 9) was reacted sequentially with samples from boring CJ-205 from the 40-, 105-, 170-, 235- and 300-ft depths. Similar to the simulation of horizontal transport, pH values progressively increase with increased reaction. Progressive increases also occurred in the Cl, Na, SO_4, and U concentrations. Decreasing trends occur in alkalinity and possibly NH_3-N. Dissolved U concentrations increased despite lowered concentrations of dissolved carbonate (alkalinity). Some carbonate was apparently lost from the solution because of outgassing and/or mineral precipitation. The progressively higher U concentrations may simply be caused by desorption from fresh adsorption sites at each reaction step, or may be caused by variable pH and pCO_2 values.

Table 13. Results of Sequential Batch-Leaching Tests

Depth (ft)	pH	ORP (mV)[a]	Cond.[b] (µS/cm)	Ca (mg/L)	Na (mg/L)	Mg (mg/L)	K (mg/L)	Alk[c] (mg/L)	Cl (mg/L)	NO_3 (mg/L)	SO_4 (mg/L)	NH_3-N (mg/L)	U (µg/L)
CJ-203, -204, and -206													
40	7.66	196.7	29400	320	5700	440	141	560	1026	764	18676	1700	5.5
40	7.79	186.3	30100	350	5400	510	156	450	1096	828	19872	1500	19.3
40	7.83	175.2	29900	349	6300	300	177	560	1120	820	19910	1300	25.4
CJ-205													
40	7.73	187.3	29200	236	5700	210	141	620	1106	756	18504	1600	3.0
105	7.85	171.4	29800	220	6400	200	168	560	1116	770	18828	1400	19.5
170	7.96	171.5	29600	199	6500	250	157	520	1196	776	19032	1100	29.0
235	7.85	173.3	29700	203	7000	180	167	400	1284	804	19700	1800	44.9
300	7.97	173.5	30600	196	7800	180	166	330	1336	794	19492	900	54.5

[a]mV = millivolt.
[b]Cond. = electrical conductivity in microsiemens per centimeter (µS/cm).
[c]Alk = alkalinity in milligrams per liter as $CaCO_3$.

Another outcome of the sequential batch-leaching tests was an estimate of the amount of labile U in the Mancos Shale. The labile U concentration is the readily releasable portion and is needed to calculate uranium R_d values as discussed in Section 6.0. Labile U should be measured using a solution that strongly favors partitioning of U into the liquid phase, such as the strong carbonate solution used by Davis and Curtis (2003). SPF-1 has a relatively high carbonate concentration and should produce a reasonable estimate of labile U; however, our results should be considered as minimum values. The labile U concentrations range from 0.0120 to 0.0660 µg/g, with a mean of 0.0436 µg/g (Table 14).

Table 14. Labile U Concentrations

Sample ID	SPF-1 (mL)	Mass (g)	U (µg/L)	Labile U (µg/g)
CJ-203-40	400	100	5.5	0.0220
CJ-204-40	315	78.75	19.3	0.0552
CJ-206-40	240	60	25.4	0.0244
CJ-205-40	400	100	3	0.0120
CJ-205-105	315	78.75	19.5	0.0660
CJ-205-170	240	60	29	0.0380
CJ-205-235	165	41.25	44.9	0.0636
CJ-205-300	100	25	54.5	0.0384
Mean				0.0436

8.0 Reaction-Transport Modeling

8.1 Introduction

This task consists of developing a reaction transport model using the PHREEQC code (Parkhurst and Appelo 1999). Ion exchange is modeled using data from the CEC determinations (Section 3.0) and surface area measurements (Section 5.0). Initial conditions include concentrations of minerals as estimated from the soluble chemistry results (Section 2.0) and XRD results (Section 4.0). A surface-complexation model (SCM) for U was developed and calibrated against the uranium R_d measurements provided in Section 6.0.

The reaction-transport model includes one-dimension transport of tailings water through the Mancos Shale. Aqueous speciation reactions are typically fast with respect to ground water flow and were modeled at chemical equilibrium. Water-to-rock interaction includes mineral precipitation and dissolution, adsorption, and cation exchange. For the models used in this study, it is assumed that the system is oxidized; no reduced species were included. Results from the sequential batch reaction tests were used to test and calibrate the reaction-transport model. Input files for the sequential batch models are presented in Appendix F. Input files for the Crescent Junction models are presented in Appendix G, and the thermodynamic database is presented in Appendix H.

The reaction-transport model is adaptable to allow inclusion of such factors as (1) mixing with ground water, (2) reaction kinetics, and (3) changing oxidation-reduction state (e.g., due to biologic activity). Thus, sensitivity of the transport to various parameters can be readily estimated with additional model simulations. In this section, each "module" of the reaction-transport model is discussed separately, and input parameters used in the reaction-transport modeling are specified.

8.2 Aqueous Speciation Module

The aqueous speciation reactions used in this study are identical to those used by Davis and Curtis (2003), supplemented with reactions in the PHREEQC.dat thermodynamic database provided with the PHREEQC program (Parkhurst and Appelo 1999). All aqueous U species are from Davis and Curtis (2003). Table 15 and Table 16 provide lists of the non-U-bearing and U-bearing aqueous speciation reactions respectively, used in this study.

Table 15. Non-U-Bearing Aqueous Speciation Reactions and Logarithmic Equilibrium Constants Used in the Reaction-Transport Modeling[a]

Reaction	Log K
$CO_3^{-2} + H^+ = HCO_3^-$	10.329
$SO_4^{-2} + H^+ = HSO_4^-$	1.98
$NH_4^+ = NH_3(aq) + H^+$	–9.252
$Ca^{+2} + H_2O = CaOH^+ + H^+$	–12.78
$Ca^{+2} + CO_3^{-2} + H^+ = CaHCO_3^+$	11.435
$Mg^{+2} + H_2O = MgOH^+ + H^+$	–11.44
$Mg^{+2} + H^+ + CO_3^{-2} = MgHCO_3^+$	11.399
$Na^+ + H_2O = NaOH(aq) + H^+$	–14.18
$Na^+ + HCO_3^- = NaHCO_3(aq)$	–0.25
$K^+ + H_2O = KOH(aq) + H^+$	–14.46
$CO_3^{-2} + 2H^+ = CO_2(aq) + H_2O$	16.683
$H_2O = OH^- + H^+$	–14.0
$NH_4^+ + SO_4^{-2} = NH_4SO_4^-$	1.11
$Ca^{+2} + CO_3^{-2} = CaCO_3(aq)$	3.224
$Ca^{+2} + SO_4^{-2} = CaSO_4(aq)$	2.3
$Mg^{+2} + CO_3^{-2} = MgCO_3(aq)$	2.98
$Mg^{+2} + SO_4^{-2} = MgSO_4(aq)$	2.37
$Na^+ + CO_3^{-2} = NaCO_3^-$	1.27
$Na^+ + SO_4^{-2} = NaSO_4^-$	0.7
$K^+ + SO_4^{-2} = KSO_4^-$	0.85

[a]From Davis and Curtis (2003) and Parkhurst and Appelo (1999).

Table 16. U-Bearing Aqueous Speciation Reactions and Logarithmic Equilibrium Constants Used in the Reaction-Transport Modeling[a]

Reaction	Log K
$UO_2^{+2} + H_2O = UO_2OH^+ + H^+$	–5.20
$UO_2^{+2} + 2H_2O = UO_2(OH)_2(aq) + 2H^+$	–11.50
$UO_2^{+2} + 3H_2O = UO_2(OH)_3^- + 3H^+$	–20.00
$UO_2^{+2} + 4H_2O = UO_2(OH)_4^{-2} + 4H^+$	–33.0
$2UO_2^{+2} + H_2O = (UO_2)_2OH^{+3} + H^+$	–2.70
$2UO_2^{+2} + 2H_2O = (UO_2)_2(OH)_2^{+2} + 2H^+$	–5.62
$3UO_2^{+2} + 4H_2O = (UO_2)_3(OH)_4^{+2} + 4H^+$	–11.90
$3UO_2^{+2} + 5H_2O = (UO_2)_3(OH)_5^+ + 5H^+$	–15.55
$3UO_2^{+2} + 7H_2O = (UO_2)_3(OH)_7^- + 7H^+$	–31.00
$4UO_2^{+2} + 7H_2O = (UO_2)_4(OH)_7^+ + 7H^+$	–21.90
$UO_2^{+2} + CO_3^{-2} = UO_2CO_3(aq)$	9.67
$UO_2^{+2} + 2CO_3^{-2} = UO_2(CO_3)_2^{-2}$	16.94
$UO_2^{+2} + 3CO_3^{-2} = UO_2(CO_3)_3^{-4}$	21.60
$3UO_2^{+2} + 6CO_3^{-2} = (UO_2)_3(CO_3)_6^{-6}$	54.0
$2UO_2^{+2} + CO_3^{-2} + 3H_2O = (UO_2)_2CO_3(OH)_3^- + 3H^+$	–0.86
$3UO_2^{+2} + CO_3^{-2} + 3H_2O = (UO_2)_3CO_3(OH)_3^+ + 3H^+$	0.66
$11UO_2^{+2} + 6CO_3^{-2} + 12H_2O = (UO_2)_{11}(CO_3)_6(OH)_{12}^{-2} + 12H^+$	36.43
$UO_2^{+2} + NO_3^- = UO_2NO_3^+$	0.3
$UO_2^{+2} + Cl^- = UO_2Cl^+$	0.17
$UO_2^{+2} + 2Cl^- = UO_2Cl_2(aq)$	–1.1
$UO_2^{+2} + SO_4^{-2} = UO_2SO_4(aq)$	3.15
$UO_2^{+2} + 2SO_4^{-2} = UO_2(SO_4)_2^{-2}$	4.14

[a]From Davis and Curtis (2003).

For this study, it was assumed that the reactions among all aqueous chemical species are at equilibrium. This assumption is reasonable because reaction rates among dissolved aqueous species are relatively fast. Numerically, this is accomplished by solving the set of Log K expressions. For example, the numerical expression for the first reaction in Table 15 is

$$Log\ K = Log\ a_{(HCO_3^-)} - Log\ a_{(CO_3^{2-})} - Log\ a_{(H^+)} \qquad \text{Equation 1}$$

where a is the activity of the dissolved species. Activities are related to concentrations using activity coefficients calculated using the Debye-Hückle theory; for example:

$$a_{(HCO_3^-)} = \gamma m_{(HCO_3^-)} \qquad \text{Equation 2}$$

where γ is the Debye-Hückle activity coefficient and $m_{(HCO_3^-)}$ is the molality of the bicarbonate ion.

8.3 Mineral Precipitation/Dissolution and Gas-Phase Module

Four minerals (calcite, gypsum, halite, and nahcolite) were allowed to equilibrate with the aqueous solution during the reaction-transport simulations. Table 17 presents these mineral reactions and their associated equilibrium constants. Similar to the aqueous speciation reactions in the previous section, equilibrium was forced between the aqueous solution and each of these minerals. Numerically, this means that the following condition must hold for each mineral, using calcite as an example:

$$Log\ K = Log\ a_{(CO_3^{-2})} - Log\ a_{(Ca^{2+})} - Log\ a_{(CaCO_3)} \qquad \text{Equation 3}$$

where $a_{(CaCO3)}$ is the activity of calcite, which is assumed to be in the pure phase and, thus, has unit activity.

Table 17. Reactions and Logarithmic Equilibrium Constants for Minerals Allowed to Equilibrate During Reaction-Transport Simulations[a]

Mineral Name	Mineral Reaction	Log K
Calcite	$CaCO_3 = CO_3^{-2} + Ca^{+2}$	–8.48
Gypsum	$CaSO_4 \cdot 2H_2O = Ca^{+2} + SO_4^{-2} + 2H_2O$	–4.58
Nahcolite	$NaHCO_3 = Na^+ + HCO_3^-$	–0.548
Halite	$NaCl = Na^+ + Cl^-$	1.582

[a]From Wateq4f.dat database supplied with the PHREEQC program (Parkhurst and Appelo 1999).

Minerals present were allowed to dissolve; therefore, the initial concentration of a mineral is an important input parameter. The initial concentrations of minerals were estimated from the NETPATH results of the water-soluble chemistry results (Table 4). The mineral compositions of samples from the 40-ft depth were distinctly different from samples from deeper depths in that they contained more gypsum and less nahcolite. Because calcite was not completely dissolved during the water extraction tests, its composition was set at 1 weight percent [0.75 mol/$L_{(gw)}$], considered to be a reasonable value for the Mancos Shale based on hand-lens observations of core samples and identification by XRD analysis. Table 18 presents the estimated mineral abundances; these values were used in the reaction-transport modeling.

Table 18. Estimated Mineral Abundances (in mole per liter of ground water) Used in Reaction-Transport Modeling

Mineral	Abundance (vertical transport)	Abundance (horizontal transport)
Calcite	0.75	0.75
Gypsum	0.02	0.50
Nahcolite	0.50	0.20
Halite	0.02	0.02

Though only the minerals listed in Table 17 were allowed to react during the transport simulations, other minerals were included in the thermodynamic database to track the saturation indices (SI). Saturation index (SI) is defined as

$$SI = \frac{IAP}{Log\ K} \qquad \text{Equation 4}$$

where IAP is the ion activity product. If the SI is positive, the solution is oversaturated, and the mineral will tend to precipitate. If the SI is negative, the solution is undersaturated, and the mineral, if present, would tend to dissolve. By tracking the mineral SI, the modeler is aware of additional mineral precipitation that may need to be included. Table 19 provides the minerals included only for information on the SI.

Table 19. Reactions and Logarithmic Equilibrium Constants for Minerals Included in Reaction-Transport Modeling but Not Allowed to Equilibrate[a]

Mineral Name	Mineral Reaction	Log K
Aragonite	$CaCO_3 = CO_3^{-2} + Ca^{+2}$	–8.336
Dolomite	$CaMg(CO_3)_2 = Ca^{+2} + Mg^{+2} + 2CO_3^{-2}$	–17.09
Anhydrite	$CaSO_4 = Ca^{+2} + SO_4^{-2}$	–4.36
Thenardite	$Na_2SO_4 = 2Na^{+} + SO_4^{-2}$	–0.179
Trona	$NaHCO_3{:}Na_2CO_3{:}2H_2O = 2H_2O + 3Na^{+} + CO_3^{-2} + HCO_3^{-}$	–0.795
Natron	$Na_2CO_3{:}10H_2O = 2Na^{+} + CO_3^{-2} + 10H_2O$	–1.311
Thermonatrite	$Na_2CO_3{:}H_2O = 2Na^{+} + CO_3^{-2} + H_2O$	0.125
Schoepite	$UO_2(OH)_2{:}H_2O + 2H^{+} = UO_2^{+2} + 3H_2O$	4.93
Rutherfordine	$UO_2CO_3 = UO_2^{+2} + CO_3^{-2}$	–14.49
Gummite	$UO_3 + 2H^{+} = UO_2^{+2} + H_2O$	10.403
Gamma UO_3	$UO_3 + 2H^{+} = UO_2^{+2} + H_2O$	7.719
Unnamed	$Na_4UO_2(CO_3)_3 = 4Na^{+} + UO_2^{+2} + 3CO_3^{-2}$	–16.290
β-$UO_2(OH)_2$	$UO_2(OH)_2 + 2H^{+} = UO_2^{+2} + 2H_2O$	5.544

[a]From Davis and Curtis (2003) and Parkhurst and Appelo (1999).

Several gas phases were also included in the thermodynamic database. The SI for a gas-phase reaction is the logarithm of its partial pressure (measured in atmospheres). Thus, by tracking the partial pressures the modeler can be aware of unusual situations, such as a partial pressure that exceeds 1 atmosphere, which could result in separation of a gas phase. Table 20 provides the three gas phases included in the modeling.

Table 20. Reactions and Logarithmic Equilibrium Constants for Gases Included in Reaction-Transport Modeling but not Allowed to Equilibrate[a]

Gas	Reaction	Log K
CO_2 (gas)	CO_2 (gas) = CO_2 (aq)	–1.472
H_2O (gas)	H_2O (gas) = H_2O (aq)	1.51
NH_3 (gas)	NH_3 (gas) = NH_3 (aq)	1.7966

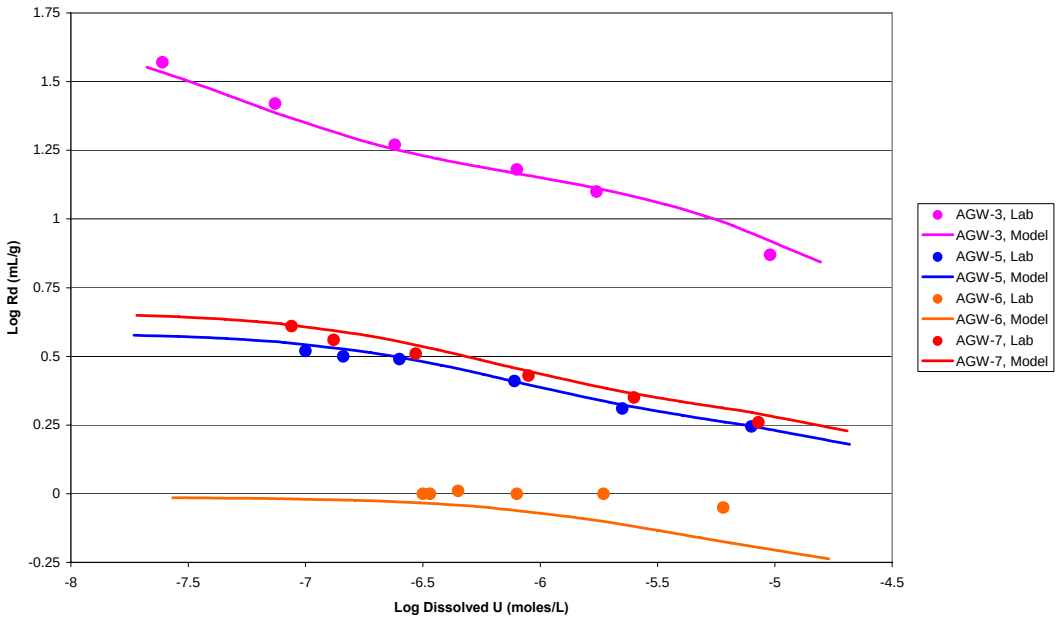
[a]CO_2 from Davis and Curtis (2003); H_2O and NH_3 from Parkhurst and Appelo (1999).
aq = aqueous

8.4 Uranium Adsorption Module

Uranium adsorption is simulated using an SCM (Davis et al. 1978). In an SCM, adsorption is a function of the electrostatic potential and the species complexation configuration at a mineral surface; these parameters vary with solution composition. The SCM approach has been widely used to model adsorption of U(VI) to pure phase minerals, in particular, iron oxyhydroxide (Davis 2001, Hsi and Langmuir 1985, Tripathi 1984, Morrison et al. 1995). Naturally occurring sediments are more complicated because of the presence of a mixture of many minerals. To simplify the use of the SCM approach in modeling field situations, Davis et al. (2004) developed an approach they called the Generalized Composite Model (GCM). In a GCM, the rock is treated as a composite of mineral phases, and surface-complexation constants for the composite are calibrated from laboratory measurements. As with the SCM, adsorption processes in a GCM vary with ground water composition. Thus, instead of treating the distribution of contaminant between solids and water as a constant (the so-called K_d approach), the K_d values vary throughout a transport simulation. To simplify computations, Davis et al. (2004) elected not to consider the effects of surface charge potential on adsorption, and we also omit this effect. Thus, the adsorption module is solved numerically using equilibrium expressions in a manner similar to the aqueous-speciation module. Three types of adsorption sites (weak, strong, and very strong) were required to produce an acceptable fit to the laboratory data.

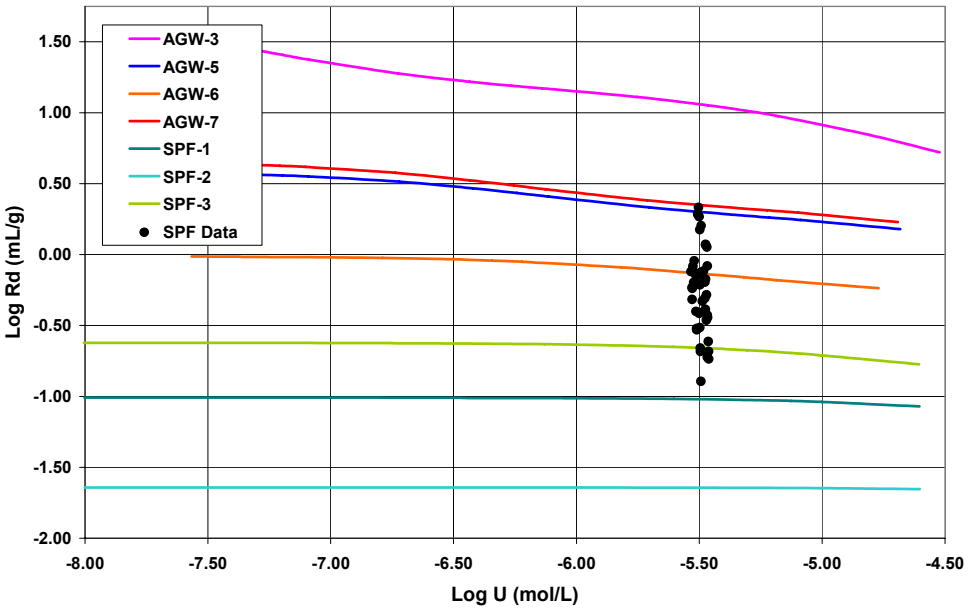
Davis and Curtis (2003) provide thermodynamic data and model parameters for a GCM. Because they used data different from that in the PHREEQC database and a different numerical processor, we started by entering their data and parameters into PHREEQC and checking the accuracy of the calculated results. The results shown on Figure 3 indicate a good match between our modeled results using PHREEQC and the laboratory results of Davis and Curtis (2003). The small differences between the PHREEQC and laboratory results for AGW-6 (Davis and Curtis 2003, label synthetic ground water as AGW) probably arise because the model is sensitive to solution parameters in this range; some of the aqueous thermodynamic data were not provided by Davis and Curtis (2003). However, the small deviation should not significantly affect the adsorption calculations for the Crescent Junction reaction-transport model.

The uranium R_d data reported in Section 6.0 were used to check the calibration of the GCM for U adsorption to Mancos Shale. By comparison with the data of Davis and Curtis (2003), the laboratory measurements from our study grouped tightly at relatively low values of R_d (Figure 4). Models of the Crescent Junction R_d measurements using the GCM, without any changes to the surface-complexation constants, are also presented on Figure 4 (SPF-1, SPF-2, and SPF-3). The R_d measurements generally plot above the models. As discussed in Section 6.0, many of the R_d measurements were negative because of variable amounts of labile U and analytical imprecision. Thus, the measured R_d values are maximum values, and the actual R_d values may be lower, as indicated by the SPF models on Figure 4. Therefore, as a first approximation, we elected to use the Davis and Curtis (2003) GCM as it is without attempting to modify the surface-complexation constants. With this approach, the uranium R_d values used for the SPF fluid migration are kept quite low, consistent with results of the R_d tests. Table 21 provides the GCM uranium adsorption surface complex reactions and associated equilibrium constants. Other input parameters needed for the GCM are proportions of weak, strong, and very strong sites = 0.9879, 0.012, and 0.0001, respectively; site density = 1.92 µmol/m^2 (Davis and Kent 1990); surface area for Mancos Shale = 11.02 m^2/g (mean value of 10 BET measurements, Section 5.0); and rock-to-water ratio = 7500 g (based on 25 percent porosity and 2.5 g/mL rock density).



Compositions of solutions AGW-3, AGW-5, AGW-6, and AGW-7 are provided in Davis and Curtis (2003).
AGW-3: pH 7.94, 0.05 percent CO_2 (lab air), 25 g/L
AGW-5: pH 7.22, 1.24 percent CO_2, 125 g/L
AGW-6: pH 6.88, 6.8 percent CO_2, 820 g/L
AGW-7: pH 7.58, 0.47 percent CO_2, 125 g/L

Figure 3. Comparison of PHREEQC Uranium Adsorption Model With Data From Davis and Curtis (2003)



SPF models use the Davis and Curtis (2003) GCM without modification.

Figure 4. Comparison of Uranium R_d Measurements (black dots) Made in This Study With Naturita Sediment Models (AGW plots) from Davis and Curtis (2003)

Table 21. Uranium Surface-Complexation Reactions and Logarithmic Equilibrium Constants Used in Reaction-Transport Modeling[a]

Reaction	Log K
$Hfo\_wOH + UO_2^{+2} + H_2O = Hfo\_wOUO_2OH + 2H^+$	–6.74
$Hfo\_sOH + UO_2^{+2} + CO_2 + H_2O = Hfo\_sOUO_2CO_3^- + 3H^+$	–8.00
$Hfo\_vOH + UO_2^{+2} + H_2O = Hfo\_vOUO_2OH + 2H^+$	–2.06
$Hfo\_vOH + UO_2^{+2} + CO_2 + H_2O = Hfo\_vOUO_2CO_3^- + 3H^+$	–6.36

[a]From Davis et al. (2004); w, s, v = weak, strong, and very strong sites.
Hfo represents an adsorption site.

8.5 Cation Exchange Module

Cation exchange was considered to be a prominent chemical mechanism for ground water transport in the Mancos Shale. The Mancos Shale contains a high proportion of clay minerals that include a significant fraction of smectite (Section 3.0. Smectites are layered silicate minerals with freely exchangeable cations within the interlayer space. The CEC was used in the reaction-transport modeling as a measure of the total amount of exchangeable sites present in the rock.

The mean CEC value of 11.23 meq/100 g (Section 3.0) was used for the modeling. The number of exchange sites in equivalents per liter (eq/L) of ground water (0.842 eq/L) was calculated as the product of the mass of rock per liter of ground water and the CEC:

$$\text{Exchange Sites} = 7500\ g_{(rock)}/L_{(gw)} * 11.23\ meq/100\ g_{(rock)} * 1\ eq/1000\ meq = 0.842\ eq/L \qquad \text{Equation 5}$$

Calculations of cation exchange by PHREEQC are accomplished by solving equilibrium expressions for each exchange reaction. For example, the exchange reaction and logarithmic equilibrium expression for Ca is

$$Ca^{+2} + 2X^- = CaX_2$$

$$Log(0.8) = Log\ a_{(CaX_2)} - Log\ a_{(Ca^{+2})} - 2Log\ a_{(X^-)} \qquad \text{Equation 6}$$

where X is on the exchange site.

Table 22 presents the exchange reactions and associated logarithmic equilibrium constants used in the modeling. Some cations have a higher selectivity for exchange sites than other cations; this selectivity is accounted for in the equilibrium constants. Retardation of NH_4 contamination from the tailings is likely to be largely a function of cation exchange.

Table 22. Exchange Reactions and Logarithmic Equilibrium Constants Used in Reaction-Transport Modeling[a]

Reaction	Log K
$H^+ + X^- = HX$	1.0
$NH_4^+ + X^- = NH_4X$	0.6
$Ca^{+2} + 2X^- = CaX_2$	0.8
$Mg^{+2} + 2X^- = MgX_2$	0.6
$Na^+ + X^- = NaX$	0.0
$K^+ + X^- = KX$	0.7

[a]From Parkhurst and Appelo (1999).
X represents an exchange site.

8.6 Model Calibration Using Sequential Batch-Leaching Results

The sequential batch-leaching results (Section 7.0) were modeled to calibrate the release of background U from the Mancos Shale and to compare modeled major-ion concentrations with experimental results. Appendix F provides the PHREEQC input files for the sequential batch-leaching simulations.

The rock-to-water ratio used in the sequential batch-leaching tests was 250 g/L (100 g of rock to 400 mL of water). Because input parameters for the models are normalized to a liter of water, the parameters for the sequential batch-leaching models are different from the field models that used a rock-to-water ratio of 7,500 g/L. Table 23 provides the normalized parameters for the sequential batch-leaching models.

Table 23. Parameters Used in Sequential Batch-Leaching Models

Parameter	Value
Rock-to-Water Ratio	250 g/L
Cation Exchange Capacity	11.23 meq/100 g
Rock Surface Area	11.02 m^2/g
Exchange Sites	0.028 eq/L
Adsorption Site Density	5290 µmol/L
Very Strong Sites	0.53 µmol/L
Strong Sites	63.5 µmol/L
Weak Sites	5226 µmol/L
Calcite Concentration	0.025 mol/L
Gypsum Concentration (40 ft)	0.01 mol/L
Gypsum Concentration (>40 ft)	0.000667 mol/L
Nahcolite Concentration (40 ft)	0.00667 mol/L
Nahcolite Concentration (>40 ft)	0.017 mol/L
Halite Concentration	0.000667 mol/L

The initial distributions of cations on the exchange sites were determined by assuming the rock sample was in equilibrium with the ground water sample collected at the Crescent Junction Site (ground water sample from Borehole 210 collected November 7, 2005). The composition of this water (Table 24) was equilibrated with the solid sample to fix the initial distribution of cations on the exchange sites.

Table 24. Composition of Borehole 210 Ground Water Collected November 7, 2005

Parameter	Value
pH	7.23
Alkalinity (mg/L as $CaCO_3$)	634
Calcium (mg/L)	180
Sodium (mg/L)	12,000
Magnesium (mg/L)	140
Potassium (mg/L)	58
Sulfate (mg/L)	1,700
Chloride (mg/L)	23,000

To calibrate the distribution of U-bearing surface adsorption complexes, the U concentration in the Borehole 210 ground water sample was adjusted until the U concentration in the model matched reasonably well with the labile U released (Table 14) during the sequential batch-leaching tests. The concentration of U required to match well with the labile U release was 0.2 mg/L. To achieve the same concentrations of U-bearing adsorption sites for the Crescent Junction reaction-transport modeling, this U concentration was scaled to 6.7 µg/L to account for the 30-fold difference in rock-to-water ratio.

After initializing the cation exchange sites and adsorption sites, a sequential batch-leaching test was simulated by reacting SPF-1 fluid with appropriate mineral phases in a step-wise fashion. For the horizontal sequential batch-leaching scenario, three reaction steps were conducted using minerals representing samples collected from the 40-ft depth Mancos Shale. For the vertical scenario, SPF-1 was first reacted with the 40-ft mineral assemblage followed by four additional reaction steps with the mineral phases representing progressively deeper Mancos Shale.

As discussed in Section 7.0, the results of the horizontal sequential batch-leaching tests showed several distinctive concentration trends. For example, concentrations of Na, SO_4, and U increased, while NH_4 decreased and Ca remained constant. These trends are simulated well with the model (Table 25). Modeled pH values were less than measured results and had a reverse trend (Table 25). Modeled alkalinity values (not listed in the table) were higher than the measured values. The inconsistencies in pH and alkalinity values are attributed largely to addition of bicarbonate ion to the solution from the dissolution of nahcolite in the model. As the bicarbonate component increases, calcite precipitates, causing pH values to decrease.

Comparison of modeled and measured results of the vertical sequential batch-leaching test shows trends similar to the horizontal scenario (Table 26). Unlike the horizontal model, pH values show an increasing trend after reaction step 3, and Ca has a decreasing trend. In both the horizontal and the vertical models, the observed trends result from interactions among several chemical processes that transfer mass between the solid and liquid phases, including mineral precipitation/dissolution, cation exchange, and specific adsorption for U. Considering the complexity of the system, the ability to simulate the measured results is quite good.

Table 25. Comparison of Measured and Modeled Results of Sequential Batch-Leaching Test for Horizontal Transport[a]

Reaction Step	pH	Ca (mg/L)	Na (mg/L)	SO_4 (mg/L)	NH_4-N (mg/L)	U (µg/L)
1	7.66 (7.01)	320 (342)	5,700 (5,941)	18,676 (19,392)	1,700 (1,707)	5.5 (8.7)
2	7.79 (6.87)	350 (344)	5,400 (6,401)	19,872 (19,517)	1,500 (1,494)	19.3 (17.1)
3	7.83 (6.78)	349 (345)	6,300 (6,836)	19,910 (19,670)	1,300 (1,301)	25.4 (25.5)

[a]Modeled results in parentheses.

Table 26. Comparison of Measured and Modeled Results of Sequential Batch-Leaching Test for Vertical Transport[a]

Reaction Step	pH	Ca (mg/L)	Na (mg/L)	SO_4 (mg/L)	NH_4-N (mg/L)	U (µg/L)
1	7.73 (6.81)	236 (347)	5,700 (5,941)	18,505 (19,123)	1,600 (1,807)	3.0 (8.9)
2	7.85 (6.74)	220 (255)	6,400 (6,631)	18,828 (19,190)	1,400 (1,580)	19.5 (17.9)
3	7.96 (6.74)	199 (185)	6,500 (7,284)	19,032 (19,248)	1,100 (1,376)	29.0 (27.0)
4	7.85 (6.76)	203 (137)	7,000 (7,905)	19,700 (19,315)	1,800 (1,194)	44.9 (36.1)
5	7.97 (6.78)	196 (105)	7,800 (8,494)	19,492 (19,382)	900 (1,033)	54.5 (45.3)

[a]Modeled results in parentheses.

8.7 Transport Modeling

Two modeling scenarios of the Crescent Junction Site are presented: (1) horizontal flow through the upper Mancos Shale (depths of less than 40-ft below ground surface) and (2) vertical flow through deeper Mancos Shale (depths greater than 40-ft below ground surface). Input files for the two scenarios are provided in Appendix G. Parameters used for the transport models are similar to those used for the sequential batch-leaching models (Section 8.6) but are scaled to account for the different rock-to-water ratio. Table 27 presents a summary of the parameter values. Modeling was conducted using the PHREEQC code (Parkhurst and Appelo 1999).

Table 27. Parameters Used in the Crescent Junction Reaction-Transport Models

Parameter	Value
Rock-to-Water Ratio	7,500 g/L
Cation Exchange Capacity	11.23 meq/100 g
Rock Surface Area	11.02 m^2/g
Exchange Sites	0.842 eq/L
Adsorption Site Density	0.1587 mol/L
Very Strong Sites	15.87 µmol/L
Strong Sites	1,904 µmol/L
Weak Sites	0.1568 mol/L
Calcite Concentration	0.75 mol/L
Gypsum Concentration (40 ft)	0.5 mol/L
Gypsum Concentration (>40 ft)	0.02 mol/L
Nahcolite Concentration (40 ft)	0.2 mol/L
Nahcolite Concentration (>40 ft)	0.5 mol/L
Halite Concentration	0.02 mol/L

8.7.1 Transport Model Setup

The horizontal flow simulation involves the flow of tailings pore fluid, represented by SPF-1 (Table 9), through shallow Mancos Shale, represented by the mineralogy of the 40-ft samples. For the vertical transport simulation, SPF-1 water flows through deeper Mancos Shale, represented by the mineralogy of samples deeper than 40 ft. For both simulations, the compositions of cation exchange sites and specific adsorption sites were set by equilibration with Borehole 210 (BH210) ground water. BH210 ground water was equilibrated with calcite and gypsum prior to equilibrating the exchange/adsorption sites. Sufficient U (6.7 µg/L) was added to BH210 ground water to match the calibration condition for composition of U-bearing surface-complexation sites determined from the sequential batch model (Section 8.6).

Transport was simulated in one dimension (similar to flow through a laboratory column or flow along a flow system streamline). The model domain consisted of 20 equally spaced cells and water flows through the domain by invoking 200 "shifts." Each shift transports water through a cell; thus, a total of 10 pore volumes (a pore volume being the volume of water within the fully saturated domain) were modeled. Pore volume is related to ground-water travel time or distance, if the ground water flow velocity is known. For simplicity, dispersion and diffusion were not included in the simulations although PHREEQC includes these capabilities.

8.7.2 Transport Model Results

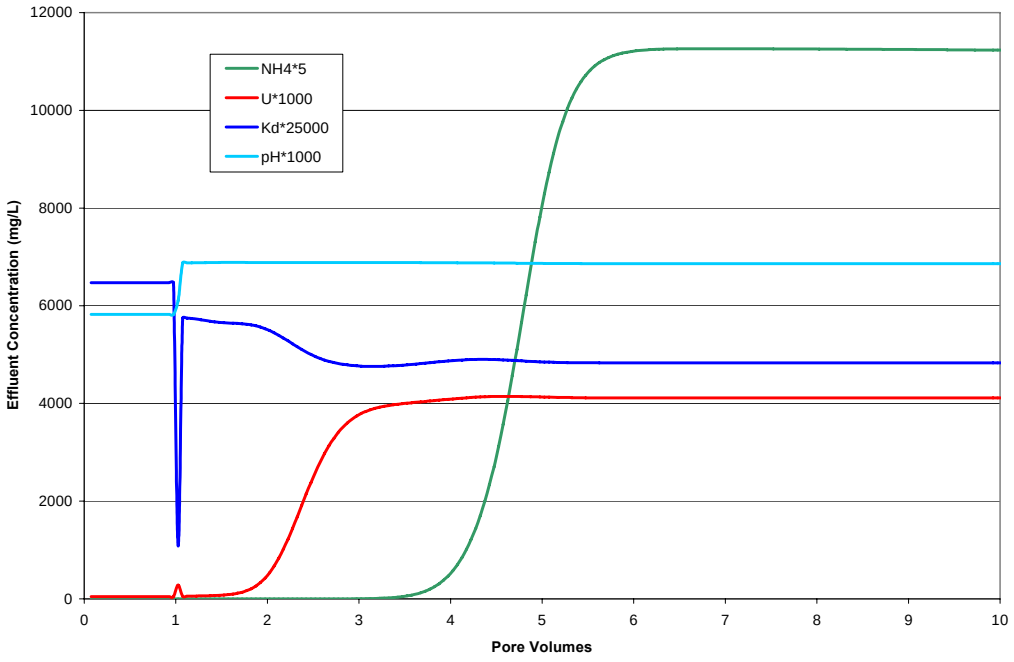
For both simulations, NH_4 is retarded for about 3.5 pore volumes, after which concentrations increase rapidly to the influent concentration (Figure 5 and Figure 6). Retardation of NH_4 is caused by the exchange of dissolved NH_4 cations for solid-phase Ca, K, Mg, and Na. Most of the exchange involves Na ions because Na dominates the cations in BH210 ground water (Table 24). Thus, the cation exchange sites on the model Mancos Shale are initially dominated by Na. The compositional variation in the cation

exchange sites caused by the different mineral assemblages in the horizontal and vertical simulations did not significantly effect retardation of NH_4.

Effluent U concentrations in the horizontal simulation are retarded for slightly less than a pore volume during which the U concentration is less than about 0.075 mg/L (Figure 5). After 1 pore volume, U concentrations increase rapidly and reach the influent value (4.0 mg/L) after about 3 pore volumes. In the vertical simulation, U concentrations are never less than 2.4 mg/L (Figure 6). However, U concentrations in the vertical simulation remain less than the influent until about 4 pore volumes.

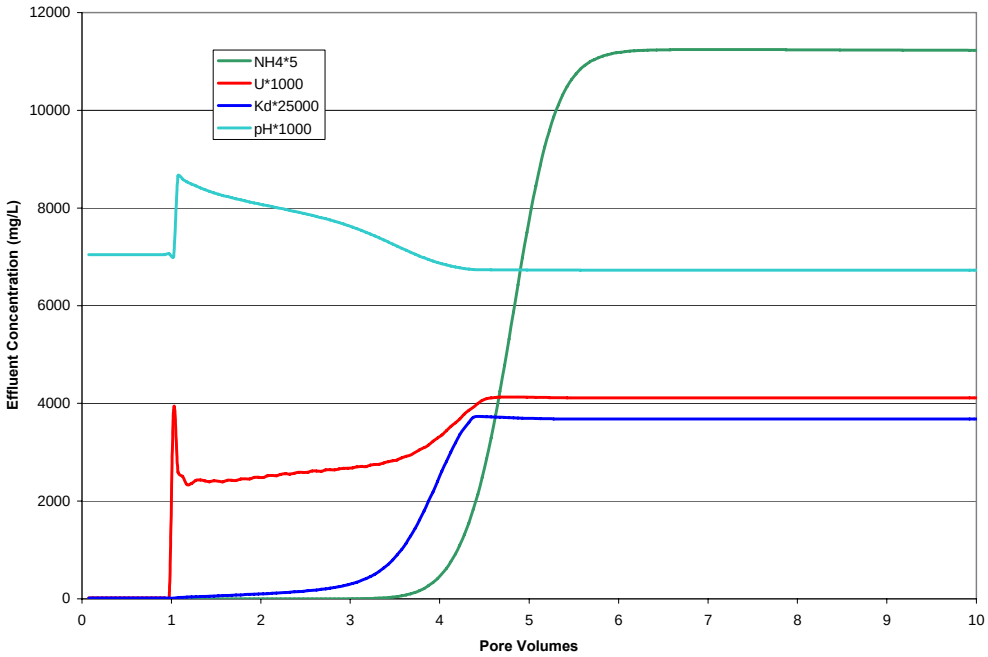
Uranium retardation is simulated by specific adsorption to the Mancos Shale. Specific adsorption is modeled using the U surface complexes listed in Table 21. Using this approach, the distribution coefficient (K_d) is not held constant but varies throughout a simulation. K_d values are not used explicitly in the simulations but were computed and are plotted on Figure 5 and Figure 6.

In the horizontal simulation, K_d values were initially 0.26 mL/g and decreased to 0.19 mL/g after about 2 pore volumes. In the vertical simulation, K_d values were negligible initially and increased to 0.15 mL/g after about 4 pore volumes. The differences in K_d values and dissolved U concentrations between the two simulations are products of the variation in the ionic composition of the solutions resulting from equilibration with minerals and cation exchange sites. A critical factor was the presence of a higher concentration of gypsum in the horizontal simulation than in the vertical simulation. Calcium released from dissolution of gypsum in the horizontal simulation caused precipitation of calcite, which resulted in decreased pH values. Initial Ca concentrations in the horizontal simulation were about 850 mg/L compared to only 9 mg/L in the vertical simulation (Figure 7 and Figure 8). These conditions led to increased partitioning of U to specific adsorption sites and increased retardation.



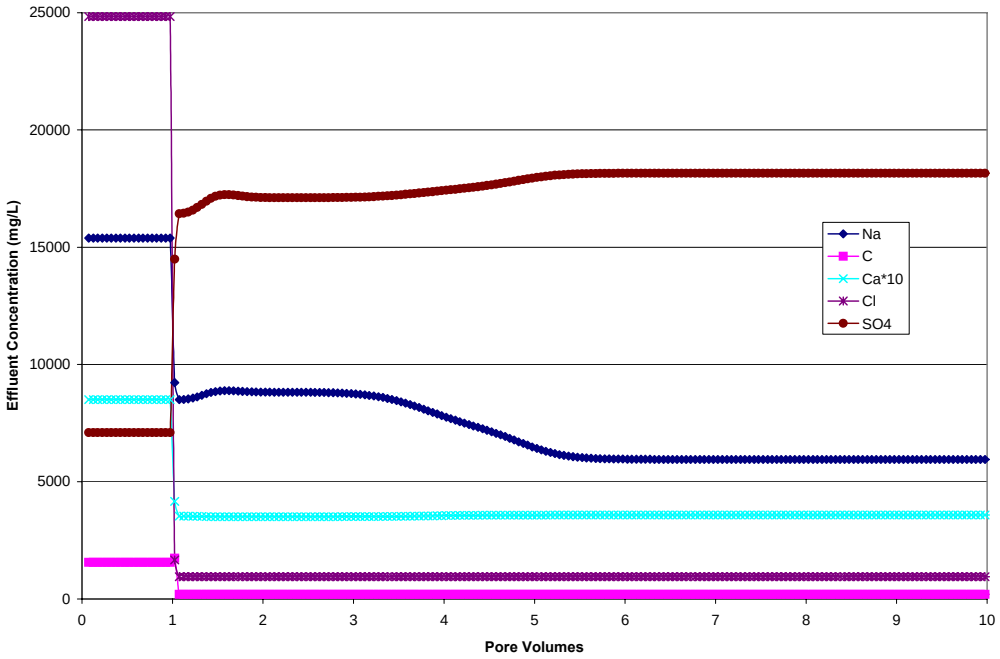
Values are scaled for plotting purposes using the multipliers shown in the legend. K_d values (mL/g) are calculated as the ratio of adsorbed concentration to dissolved concentration.

Figure 5. Effluent (Cell 20) Concentrations of U (mg/L), NH_4 (mg/L), and Uranium K_d (mL/g) and pH Values for the Horizontal Transport Simulation



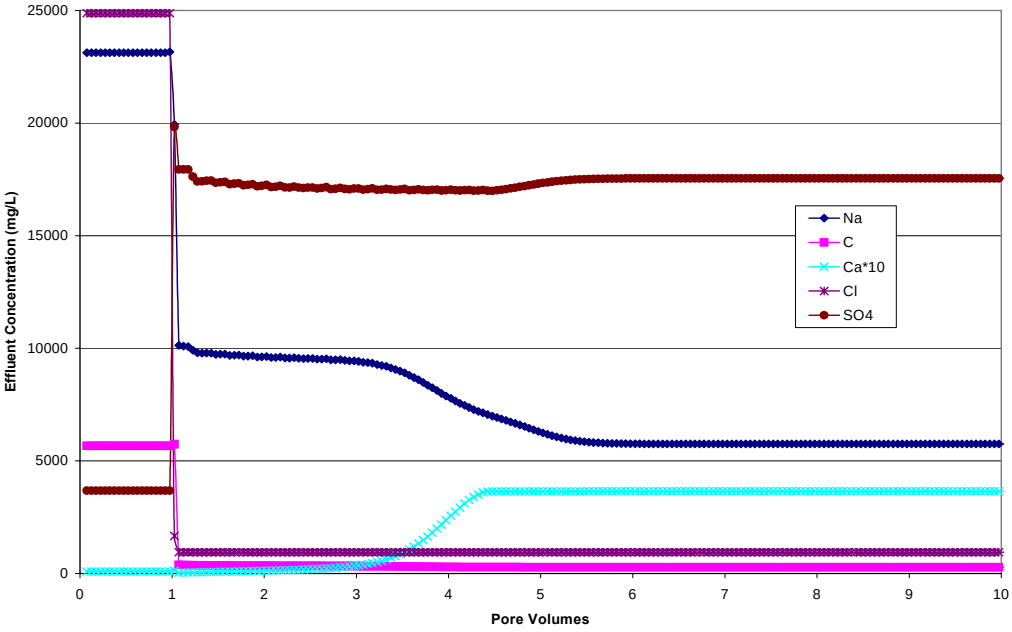
Values are scaled for plotting purposes using the multipliers shown in the legend. K_d values (mL/g) are calculated as the ratio of adsorbed concentration to dissolved concentration.

Figure 6. Effluent (Cell 20) Concentrations of U (mg/L), NH_4 (mg/L), and Uranium K_d (mL/g) and pH Values for the Vertical Transport Simulation



Calcium values are multiplied by 10 for plotting purposes.

Figure 7. Effluent (Cell 20) Concentrations of Major Ions for the Horizontal Transport Simulation



Calcium values are multiplied by 10 for plotting purposes.

Figure 8. Effluent (Cell 20) Concentrations of Major Ions for the Vertical Transport Simulation

Elevated initial SO_4 concentrations in the horizontal simulation are caused by gypsum dissolution, and lower initial dissolved carbon (IV) concentrations result from calcite precipitation. Chloride concentrations are similar between the two simulations because it was treated as a conservative ion with no chemical reactions to affect it.

In summary, the transport results suggest that NH_4 migration is retarded by several pore volumes. Uranium is retarded by about 1 pore volume but only if Ca is released from gypsum dissolution.

It is beyond the scope of this investigation to estimate ground water velocity beneath the proposed disposal cell at the Crescent Junction Site; thus, results of the model simulations were provided in terms of pore volumes. To use these results in a field setting, units of pore volume must be converted to more useful units of travel time and distance. The conversion is straightforward if the ground water velocity is known. For example, if the ground water flows horizontally from the disposal cell at 10 ft per year, the projected concentrations of U and NH_4 at a distance of 10 ft after 1 year are equivalent to the values at 1 pore volume on Figure 5. For the same ground water flow velocity at a distance of 5 ft, the projected concentrations are equivalent to 2 pore volumes after 1 year. After 2 years, the concentrations at the 10-ft and 5-ft distances are equivalent to 2 and 4 pore volumes, respectively, and so on. If the porosity of the Mancos Shale aquifer is significantly different than the value (0.25) used in the simulations, then model input would need to be reformulated. Thus, if ground water moves dominantly by fracture flow, some modifications will likely be required.

8.8 Model Limitations

The models presented in the previous section couple many of the chemical processes that are likely to affect transport of constituents at the Crescent Junction Site. Model limitations include both hydrologic and chemical factors. Importantly, the model is *not* limited by an assumption of a constant distribution coefficient (K_d) for U, an assumption that has been questioned by Davis et al. (2004).

Ground water flow modeling with PHREEQC is limited to one dimension. Thus, models are constrained to a single streamline. Although the modeling code is able to simulate dispersion and diffusion, these processes were not included for simplification purposes. Because of the low-bulk hydraulic conductivity, much of the ground water transport through the Mancos Shale is likely to be through fractures or other

large-scale features. Such features are not explicitly considered in the models presented in this study. Rather, the flow regime is implicit by the values used to assign concentrations of minerals, exchange sites, and adsorption sites. Because we based these values on the results of laboratory determinations of surface area and bulk density, we made an implicit assumption of pseudo porous-media flow. Adaptation of the model to fracture flow would be accomplished by decreasing the concentrations of sites and minerals (normalizing to a liter of ground water).

The ionic strength of the tailings pore fluids is higher than is commonly prescribed as a limit for use of the Debye-Hückle theory used in PHREEQC to calculate activity coefficients. The ionic strength limitation could be improved by employing empirical activity coefficient algorithms, such as the Pitzer equations (Mariner 2001). Unfortunately, these activity models exist for some of the major ions but are not available for U.

As a first approximation, oxidation-reduction (redox) processes were ignored in the transport models. Although the PHREEQC code is capable of calculating redox equilibria, many redox processes are rate limited. Rate-limited processes can be incorporated in PHREEQC, but universally applicable kinetic data needed to apply these processes are currently unavailable. Another reason for omitting redox processes in the models is that no data are available to confirm that redox processes are occurring in the Mancos Shale at the Crescent Junction Site. Scattered occurrences of pyrite and carbonaceous material suggest that redox processes could be occurring. However, some data suggest relatively oxidized conditions as deep as 300 ft (the depth of the boreholes at the site). Ground water collected from six of these boreholes has redox potentials ranging from 234 to 442 millivolt (mv) with one exception of 15 mV (SEEPro database). The two values of dissolved oxygen that were determined on these same ground water samples have values (2.41 mg/L and 2.8 mg/L) consistent with oxidized conditions. Also, scattered occurrences of oxidized iron (limonite) staining are present in the upper portion of the Mancos Shale. If data collected later confirm the presence of redox processes, these processes are readily stimulated by the reaction-transport model.

Other chemical factors that limit the modeling are omission of solid solutions and rate-limited processes. These are omitted from the working model because of lack of data to support a viable analysis rather than lack of model capabilities.

9.0 Conclusions

The water-soluble mineral assemblage of the Mancos Shale at the Crescent Junction Site is likely dominated by nahcolite with major amounts of Ca-Na exchange and gypsum. Halite, sylvite, and dolomite occur in lesser amounts and calcite is present. Gypsum and dolomite are more dominant in the shallow samples, while nahcolite and halite are more concentrated in the deeper samples. Cation exchange capacity of the Mancos Shale ranges from 0.54 to 36.29 meq/100 g with a mean of 11.23 meq/100 g. The bulk mineral assemblage in the Mancos dominated by quartz, with lesser amounts of dolomite and calcite, small amounts of feldspar, and traces of gypsum. The clay mineral fraction is dominated by mixed-layer (mostly illite/smectite) clays, illite, and kaolinite with illite layers dominating the mixed-layer clays. Particle surface area ranges from 8.81 to 13.22 m^2/g with a mean of 11.02 m^2/g. Distribution ratios for uranium adsorption on Mancos Shale are low, ranging from essentially 0 to 0.84 mL/g.

As tailings fluids reacted with progressively more Mancos Shale in sequential batch tests, slight increases were observed in pH, and concentrations of Na, K, Cl, SO_4, and U. Results of a reaction-transport model of sequential batch tests showed reasonably good agreement with observed concentrations for Na, Ca, SO4, NH_4, and U, but the modeled pH values were slightly less than the observed values. Considering the complexity of the chemical interactions, these results were considered favorable; thus, this model was used in a one-dimensional simulation of contaminant transport beneath the Crescent Junction disposal cell. The transport results suggest that NH_4 migration is retarded by several pore volumes. Uranium is retarded by about 1 pore volume, but only if Ca is released from gypsum dissolution. To evaluate the effects of this analysis on contaminant transport beneath the proposed Crescent Junction disposal cell, it is necessary to know the flux of contaminated water from the cell and the effective porosity of the Mancos Shale. Evaluation of the flow regime was beyond the scope of this investigation; thus, results of the model simulations are provided in terms of pore volumes. To maximize the benefit of these results in the field setting, project personnel will need to couple these results given in units of pore volume, with the results

from hydrologic investigations to yield more useful units of travel time and distance. Alternatively, a sensitivity analysis that uses reasonable bounds for the hydrologic parameters may be appropriate to assess the impact of chemical attenuation at the Crescent Junction Site.

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End of current text

Appendix A

Copy of "Work Plan Geochemical Analysis of Mancos Shale Cores from the Crescent Junction Disposal Cell Site"

DOE EM/GJ1118-2006

Work Plan
Geochemical Analysis of Mancos Shale Cores from the Crescent Junction Disposal Cell Site, Moab UMTRA Project

January 2006

Work Performed by S.M. Stoller Corporation under DOE Contract No. DE–AC01–02GJ79491
for the U.S. Department of Energy Office of Environmental Management,
Grand Junction, Colorado

Contents

1.0 Introduction 1
2.0 Task Descriptions 1
2.1 Task 1 – Preparation and Sample Collection 2
2.2 Task 2 – Analysis of Water Soluble Fractions 2
2.3 Task 3 – Measurements of Cation Exchange Capacity (CEC) 3
2.4 Task 4 – X-ray Diffraction Analysis 4
2.5 Task 5 – Determine Surface Area of Mancos Shale 4
2.6 Task 6 – Determination of Distribution Ratios 4
2.7 Task 7 – Sequential Batch Leaching Test 5
2.8 Task 8 – Coupled Hydrogeochemical Transport Modeling 6
2.9 Task 9 – Reporting 6
3.0 Schedule 6
4.0 References 6

Tables

Table 1. Analytical Methods 2

1.0 Introduction

This work plan details work that will be done to characterize the geochemistry of the bedrock beneath and adjacent to the proposed disposal cell at Crescent Junction, Utah. The disposal cell will contain tailings from the Moab, Utah, (Atlas) uranium mill and will be underlain by Mancos Shale Formation. The purpose of the work is to provide data that will help evaluate the potential for ground water contamination and transport by constituents in the tailings. The basis for this work is provided in Section 4.5 of Department of Energy (DOE) (2005) and has been modified based on discussions with Moab UMTRA Project personnel. The scope includes laboratory investigation and geochemical modeling, and is presented as nine individual tasks.

The geochemical approach involves collecting site-specific data that can be used to model geochemical interactions between tailings pore fluid and the Mancos Shale. Results from this work will provide the following information about the Mancos Shale:

- Abundance and mineralogy of water soluble minerals
- Mineralogy of water insoluble minerals, including clay mineralogy
- Cation exchange capacity
- Surface area
- Chemical distribution ratios (R_d)

The data will be used to construct a one-dimensional coupled hydrogeochemical model of tailings water transport through the Mancos. The model will include equations governing aqueous speciation, mineral dissolution, mineral precipitation, mixing with other ground water, oxidation/reduction, cation exchange, and adsorption. In addition, a sequential batch-leaching test will be conducted and the results used to help calibrate the geochemical model. Numerous analyses of tailings pore fluids have been made previously and no additional analyses will be made for the current work scope.

Samples of Mancos Shale will come from 10 cores that were collected from borings evenly distributed in the area of the proposed disposal cell (see DOE 2005 for locations). Samples will primarily consist of the Blue Gate Shale Member of the Mancos Formation because this unit is the most likely to receive contaminated drainage from the disposal cell. Some samples may also be collected from the Prairie Canyon Member of the Mancos. Approximately five samples will be collected from each of the 10 cores for a total of 50 samples. The disposal cell will be excavated approximately 20 ft into the ground; thus, the uppermost sample will be collected from a depth of about 40 ft. The remaining four samples (per core) will be collected at equal intervals below 40 ft. These samples should provide a reasonable set of data to evaluate lateral and vertical distribution of geochemical properties in the Mancos.

2.0 Task Descriptions

This section provides details of the nine individual laboratory and modeling tasks. The laboratory portion of the work will be conducted in the Applied Sciences and Technology (AST) testing

facility at the Grand Junction site. Equipment available in the AST facility that will be used for this work include:

- Ion chromatograph
- PH/ORP/conductivity probes and meters
- Balances
- Shaker tables
- Atomic absorption spectrometer
- Solids/liquid separation equipment
- Drying ovens
- Specialized spectrometers and other sample analysis equipment

A subcontract will be procured with Mesa State College to conduct X-ray diffraction (XRD) analysis. Particle surface areas using BET will be measured by a contract laboratory. Analytical methods are presented in Table 1.

Table 1. Analytical Methods

Constituent	Procedure Number DOE (2005b)	Procedure Description
Alkalinity	AP(Alk-1)	Titration with H_2SO_4
Ammonia	AP(NH_3-1)	Spectrometry - Salicylate
Calcium	AP(Ca-1)	Flame Atomic Absorption
Chloride	AP(Cl-2)	Ion Chromatography
Magnesium	AP(Mg-1)	Flame Atomic Absorption
Nitrate	AP(NO_3-4)	Ion Chromatography
Oxidation/Reduction Potential	AP(ORP-1)	Electrode
pH	AP(pH-1)	Electrode
Potassium	AP(K-1)	Flame Atomic Absorption
Sodium	AP(Na-1)	Flame Atomic Absorption
Specific Conductance	AP(EC-1)	Electrode
Sulfate	AP(SO_4-4)	Ion Chromatography
Uranium	AP(U-2)	Kinetic Phosphorescence

2.1 Task 1 – Preparation and Sample Collection

Task 1 includes procurement of chemicals and supplies, many of which are already available in the AST testing facility. Subcontracts with Mesa State College for XRD analysis and a contract laboratory for BET analysis will be procured.

Five samples will be collected from each of the 10 cores. The samples will be collected at depths of 40 ft, 105 ft, 170 ft, 235 ft, and 300 ft. Each sample will contain approximately 3 linear inches of core. Samples will be air-dried and stored in plastic containers until used for the tests. A sample log will be prepared that contains sample numbers, bulk weights, and moisture contents. Dried samples will be lightly crushed with a hammer or pestle, sieved, and split using a riffle splitter as needed for the tests.

2.2 Task 2 – Analysis of Water Soluble Fractions

Task 2 is designed to identify and estimate abundance of minerals present in the water-soluble fraction of the Mancos. Mineral identification will be aided by the XRD work in Task 4; however, XRD is limited in its ability to detect small amounts (less than about 5 percent) of

mineral and does not provide information on mineral abundance. All 50 samples will be analyzed. Water-soluble minerals are likely to include thenardite (Na_2SO_4), halite (NaCl), gypsum ($CaSO_4.2H_2O$), and other Na-Ca-K-Mg-SO_4-CO_2-NO_3-Cl-bearing salts. Analyses will include major ions that make up these minerals as well as mill tailings contaminants NH_3 and U.

Samples will be crushed, air dried, and sieved to –10 +18 mesh (1 to 2 mm nominal diameter). The size fraction was selected because: (1) it is likely to have sufficient material to accomplish the testing, (2) it is uniform enough so that surface area is relatively constant and easy to determine, and (3) it is efficient to work with in the laboratory (testing apparatus can be relatively small).

The leaching procedure is modified from DOE 2005b, procedure CB (BT-1). Two grams of the sieved sample is placed in a plastic centrifuge tube with 100 mL of deionized water at room temperature. The tube is agitated end-over-end for four hours. The solids are separated from the water by centrifuging and decanting, and/or filtering to produce a clear solution. The solution is then analyzed for pH, ORP, specific conductance, alkalinity, Ca, Na, Mg, K, SO_4, Cl, NO_3, NH_3, and U.

The solid-phase concentration of each leachable major ion will be calculated from the measured concentration and the solid/solution masses used. These solid-phase concentrations will be cast in mole units and mineral stoichiometry will be used to estimate abundances of soluble minerals. The geochemical computer program NETPATH (Plummer et al., 1994) may be used to help determine possible mineral mixtures. In NETPATH, the user can define the initial solution by the composition of the test leachate and the final solution as pure water. Various combinations of mineral phases can be specified and the program calculates the amount of each phase that must precipitate to meet the compositional constraints. Results of X-ray diffraction will help to identify possible mineral phases. Solid-phase concentrations of the contaminants NH_3 and U will also be calculated; however, concentrations are expected to be small and identification of the mineral phases containing these constituents will not likely be possible.

2.3 Task 3 – Measurements of Cation Exchange Capacity (CEC)

The Mancos Shale contains abundant clay minerals. Many types of clay have large CEC that can cause significant changes to ground water chemistry. Knowledge of the CEC is required to develop a geochemical model of water rock interactions. Therefore, CEC will be measured on 20 core samples of Mancos.

Samples will be crushed, air dried, and sieved to –10 +18 mesh (1 to 2 mm nominal diameter) in the same manner as for other tests. The CEC will be determined using a standard method such as the Ca/Mg exchange method (Jackson, 1969) or the ammonium saturation method (Chapman, 1965 as described in Bain and Smith, 1987). The choice of method will be determined after a thorough review of the applicability to the Mancos cores. For the Ca/Mg exchange method, approximately 0.5 to 2 g (exact weight depends on expected CEC) of Mancos is saturated with Ca^{2+} using 0.5 N $CaCl_2$ solution. The Ca^{2+} ion is then replaced with Mg^{2+} using 0.5N $MgCl_2$, and the concentration of Ca^{2+} released is used to calculate CEC. For the ammonium saturation method, the clay sample is first saturated with ammonium ion using one molar ammonium acetate followed by exchange with sodium chloride. CEC will also be measured on one powdered Mancos sample to provide information on maximum CEC.

2.4 Task 4 – X-ray Diffraction Analysis

Chemical interaction between ground water and Mancos Shale is likely to occur mostly at the surfaces of clay minerals. Therefore, clay mineral chemistry is important to the transport of contaminants by the ground water. XRD is one of the best analytical tools to identify the mineralogy of the clay mineral fraction of the Mancos. Ten core samples will be selected for XRD analysis.

Mancos samples will be finely powdered with a mortar and pestle and fractions will be separated by suspension in Calgon solution to concentrate the clay minerals. These clay-mineral separates will be treated in four different ways prior to XRD analysis (Wilson, 1987): (1) air dried, (2) glycolated, (3) heated 300 °C, and (4) heated 550 °C. XRD patterns from these runs will be used to identify clay minerals such as illite (I), smectite (S), interlayered I/S, chlorite, and kaolinite.

X-ray diffraction (XRD) will also be used to determine the major minerals present in the core samples. For these analyses, the 10 core samples will be powdered and oriented randomly.

2.5 Task 5 – Determine Surface Area of Mancos Shale

Knowledge of the surface area of the Mancos Shale samples used in the testing is needed to relate the results to the transport of contaminants through the subsurface. Processes such as cation exchange and adsorption are directly related to the surface area that the ground water contacts. For example, for the same travel distance, interaction of dissolved contaminants with the rock will be much less in a fracture-dominated matrix than for porous-media flow. It is beyond the scope of this work plan to determine the nature of the flow (fracture-verses-porous media) in the subsurface at the Crescent Junction site; however, to properly use the data collected during this study in site models, they will need to be normalized to surface area. Therefore, it is important to measure the surface area of the samples used in the testing.

Surface area will be determined for a subset of 10 core samples. Samples will be crushed, air dried, and sieved to –10 +18 mesh (1 to 2 mm nominal diameter) in the same manner as for other tests. Surface area will also be measured on a powdered Mancos sample to provide information on maximum surface area. Surface area will be determined by the standard Brunauer, Emmett, and Teller (BET) method. This method uses N_2 gas adsorption isotherms at –183 ^{o}C to measure surface area (Jackson 1969).

2.6 Task 6 – Determination of Distribution Ratios

Distribution ratios (R_d) provide a measure of the partitioning of a contaminant between the ground water and the solid constituents that comprise the aquifer. The higher the R_d, the more partitioning to the solids and the more retardation. The R_d value is an empirical value that is simply the ratio of the measured concentration in the solids (mg/kg) to the measured concentration in the ground water (mg/L) and has units of mL/g. The R_d values are often used to simulate retardation of contaminants in ground water models. When used in these models there is an implicit assumption that chemical retardation occurs by the process of adsorption under equilibrium conditions. For the equilibrium assumption, the R_d value is often referred to as a

K_d value. Many models also assume that K_d does not vary with the concentration of the contaminant. However, research has shown that this variation sometimes exists and algorithms such as the Langmuir or Freudlich equations are used to produce a better fit to the R_d data. To test if R_d varies with contaminant concentration, multiple points using various concentrations are measured and plots of these "adsorption isotherms" are fitted with the various models. If the plot is reasonably linear, then a K_d (also termed linear isotherm) will produce satisfactory results.

R_d values will be determined using DOE (2005b) procedure CB (Rd-1). In summary, a sample of Mancos Shale is crushed and sieved to –10 +18 mesh (1 to 2 mm nominal diameter) as in Task 2. The sample (5 g) is placed in a plastic centrifuge tube with 100 mL of synthetic pore fluid (SPF) that simulates tailings pore fluid. The R_d value can vary significantly with solution chemistry. For example, Davis et al. (2004) showed that R_d values for U in a sample of alluvium varied by more than a factor of 10 depending on dissolved carbonate concentration and pH value. R_d values will be determined using three SPF compositions that are designed to simulate ground water that could be present in the Mancos Shale after construction of the disposal cell. One solution (SPF-1) will simulate pore fluids that currently exist in the tailings. Another solution (SPF-2) will simulate tailing pore water mixed with 50% Mancos ground water. A third solution (SPF-3) will simulate water that results from the sequential batch-leaching test discussed in Task 7.

Single-point R_d measurements for U will be made on 20 samples and 6-point isotherms will be measured on five of these using SPF-1. For the five samples used for isotherms, single-point R_d values will also be determined using SPF-2 and SPF-3 to evaluate sensitivity to solution chemistry. The R_d approach is only valid for contaminants that occur in trace concentrations. Due to the high concentrations present in the pore fluid, modeling the transport of NH_3 by adsorption is not valid; thus, R_d values for NH_3 will not be measured.

2.7 Task 7 – Sequential Batch Leaching Test

Two sequential batch-leaching tests will be conducted to "measure evolution of tailings leachate", chemistry as it interacts with Mancos Shale. For this study, it is assumed that the major transport path is either vertically downward beneath the tailings pile or subhorizontal through the weathered zone. Results of this test will be used to help validate the coupled hydrogeochemical transport model presented in the next section.

For the vertical scenario, a 100-g sample of Mancos (40-ft depth) will be crushed, air dried, and sieved to –10 +18 mesh (1 to 2 mm nominal diameter). The sample will be combined with 400 mL of SPF-1 in a 500-mL glass Erlenmeyer flask. The mixture will be agitated on an orbital shake table for 24 hours. At that time, the solids will be separated from the liquid by centrifugation, decantation, and/or filtering. A 50-mL split will be retained and analyzed for pH, ORP, specific conductance, alkalinity, Ca, Na, Mg, K, SO_4, Cl, NO_3, NH_3, and U. The remaining solution will be placed with approximately 87.5 g of Mancos sample from 105-ft depth. The exact amount of Mancos sample will be calculated so the water-to-rock ratio remains constant. The procedure will be repeated three times with progressively deeper samples.

For the horizontal scenario, a 3-step leach will be conducted using the 40-ft deep samples from cores 203, 204, and 206.

2.8 Task 8 – Coupled Hydrogeochemical Transport Modeling

This task consists of developing a coupled hydrogeochemical transport model using the PHREEQC code (Parkhurst and Appelo, 1999). Ion exchange will be modeled using data from the CEC tests in Task 3 and surface area measurements in Task 5. Initial conditions will include concentrations of minerals as estimated from the results of Tasks 2 and 4. A surface complexation model for U, based on R_d measurements (Task 6) will be incorporated.

The model will include one-dimension transport of tailings water through the Mancos Shale. Aqueous speciation reactions are typically fast with respect to ground water flow and will be modeled at chemical equilibrium. Water-rock interaction will include mineral precipitation and dissolution, adsorption, and cation exchange. The model will be adaptable to allow inclusion of such factors as: (1) mixing with ground water, (2) reaction kinetics, and (3) changing redox state (e.g., due to biologic activity). Thus, sensitivity of the transport to various parameters can be readily estimated with additional model simulations. Two model simulations will be conducted to simulate the vertical and horizontal scenarios described in Section 2.7. The model can be used to simulate other transport paths with minor changes.

2.9 Task 9 – Reporting

Results of the testing and modeling will be presented as Moab Calculation Sets.

3.0 Schedule

Completion Date	Activity
January 13, 2006	Task 1. Preparation and Sample Collection
March 4, 2006	Task 2. Analysis of Water Soluble Fractions
March 4, 2006	Task 3. Measurements of Cation Exchange Capacity
March 4, 2006	Task 4. X-Ray Diffraction Analysis
March 4, 2006	Task 5. Determine Surface Area of Mancos Shale
March 4, 2006	Task 6. Determination of Distribution Ratios
March 4, 2006	Task 7. Sequential Batch Leaching Test
May 10, 2006	Task 8. Coupled Hydrogeochemical Transport Modeling
June 1, 2006	Task 9. Draft Report

4.0 References

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Appendix B

Laboratory Notes

AMPAD EFFICIENCY LINE® 22-210

CJ01-01-01

Crescent Jctn. Task 1 Sample Collection

1/9/06

Travel to Crescent Junction site to obtain core samples with Shannon and C Doodknight.

Appropriate core boxes retrieved from sea-land storage. An approx 3" piece of core was obtained @ the bedel noted with the top of the core starting @ the level noted eg. 201-40 = 201-40' to 40'9".
Larger split of CJ205-40 obtained for addtl testing
Samples were split off w/ chisel and hammer when there was no natural weak line. Spacers were placed in coreboxes to indicate sample locations

Samples were double bagged and labelled for return to GJO.

Samples were delivered to Geotech Engineering Group for prep with following instruction
1. Do not pulverize
2. Gently disaggregate to -10/+18 (1-2mm nominal diameter)
3. Avoid (as much as possible) generating heat.
4. Once disaggregated, place in labelled, sealed ziplock bags to avoid loosing moisture content.

Samples returned to GJO. Placed in pans for air drying. LOD calculated.
Samples then sieved into 3 size fractions to obtain the 1-2 mm split for analysis

+10 mesh	= >2mm
-10/+18	= 1-2mm
-18	= <1mm

Crescent Jctn. Task 2 Water Soluble fraction

CJ01-01-02

1/17/06

Place 2g of each of the following into 50mL centrifuge tubes. Add 50mL Milliq H_2O

Sample	Size
CJ201-40	1-2 mm
105	
170	
235	
300	
CJ202-40	
105	
170	
235	
300	

Sample	Size
CJ203-40	1-2mm
105	
170	
235	
300	
CJ204-40	
105	
170	
235	
300	

Place on end over end stir bar @ 8RPM x 4 hours

Remove from stir bar. Centrifuge 30" x 3500 RPM

Decant into individual 100mL volumetric flasks.

Refill cent tubes ~ 50mL Milliq H_2O

Place on end over end stir bar @ 8RPM x 30"

Remove from stir bar, Centrifuge 30" x 3500 RPM

Add decantate to respective Vol. flask. Fill to vol ~ Milliq

Filter through 0.45 µm Vac. filter. Analyze. Results, see attached spreadsheet

Crescent Gen Task 2

CJ01-01-03

1/18/06 Place 2g ea of the following into 50 mL centrifuge tubes. Add 50mL Millig H_2O

Sample	Size
CJ205-40	1-2mm
105	
170	
235	
300	
CJ206-40	
105	
170	
235	
300	
CJ207-40	
105	
170	
235	
300	
CJ208-40	
105	
170	
235	
300	

Place on end over end stir bar @ 8RPM x 4 hours

Remove from stir bar. Centrifuge 30" x 3500 RPM

Decant into individual 100mL Volumetric flasks

Refill cent. tubes ea 50mL Millig H_2O

Place on end over end stir bar x 30" @ 8RPM

Remove from stir bar. Centrifuge 30" x 3500 RPM

Add supernatant to respective vol. flasks. Fill to vol ea Millig

Filter through 0.45 um Vac. filter. Measure parameters, analyze. See attached spreadsheet

Crescent Jan. Task 2

CJ01-01-04 3

1/19/06

Place 2g of each of the following into 50mL centrifuge tubes. Add 50mL Millig H2O

Sample	Size
CJ209-40	1-2mm
105	
170	
235	
300	
CJ210-40	
105	
170	
235	
300	

Sample	Size
CJ-202-40D	1-2mm
204-40D	
206-40D	
208-40D	

Place on end over end stir bar @ 8RPM x 4 hours

Remove from stir bar. Centrifuge 30" x 3500RPM

Decant into individual 100mL vol. flasks

Repeat cent. twice ε 50mL Millig H2O

Place on end over end stir bar @ 8RPM x 30"

Remove from stir bar, centrifuge 30" x 3500RPM

Add supernatant to respective vol flask. Fill to Vol ε Millig

Filter through 0.45μm Vac filter. Measure parameters, analyze. See attached spreadsheet

Crescent Junction CEC Task 3 CJ01-01-05

2/4/06 Place 100 mg of the following samples in 30 ml cent. tubes. Follow CB ~~AP~~ Sn (CEC) c̄ 1° exposure to amacetate x 4 then overnight for 5th soak.

	Sample	NH_3-N (mg/L)	CEC (meq/100g)
2/4/06 start	CJ201-40	0.65	9.286
	202-40	0.82	11.714
	203-40	2.54	36.286
	204-40	0.75	10.714
	205-40	0.75	10.714
	206-40	0.41	5.857
	207-40	1.08	15.429
	208-40	0.49	7.000
	209-40	1.19	17.000
	210-40	0.80	11.429
	205-40P	0.72	10.286
	205-40P-D	~~0.89~~ 0.73	~~12.714~~ 10.429
2/5/06 start	201-105	0.37	5.286
	202-105	0.80	11.429
	203-105	0.49	7.000
	204-105	0.90	12.857
	205-105	0.87	12.429
	206-105	0.52	7.429
	207-105	0.60	8.571
	208-105	0.50	7.143
	209-105	1.03	14.714
	210-105	0.38	5.429
	204-105D	0.92	13.143
	205-40D	0.89	12.714

Task 4 XRD

CJ01-01-06

1/17/06 Place ~~a~~ an approx 15g split of the following samples in individual 30ml centrifuge tubes. Samples are of the <1mm size fraction, air dried. All are from the 40' depth.

Sample

CJ-201-40
202-40
203-40
204-40
205-40
206-40
207-40
208-40
209-40
210-40

Deliver to Dr. Bill Hood for XRD analysis

Crescent Jctn. Task 5 - BET Surface Area. CJ01-01-07

1/17/06 Prepare the following samples for shipment to Micromeritics for BET method multipoint surface analysis. All are air dried from 40' below surface. Place ~ 30g of the following in 30ml cent tubes.

Sample	Particle size (mm)	
CJ201-40	+2	
202-40	1-2	
203-40	1-2	
204-40	1-2	
205-40	1-2	
205-40 P	<1	(powdered)
206-40	1-2	
207-40	1-2	
208-40	1-2	
209-40	1-2	
210-40	1-2	

Send to Micromeritics Analytical Services via Fdex
One Micromeritics Dr
Norcross, GA 30093-1877
1-770-662-3630

Request Cat #005-01 Multipoint surface area analysis - N_2 gas

2/2/06 Call Micromeritics re analysis - 1-2mm size frac results comparable to powdered sample. Confirmed samples run as submitted (not powdered) w/ phone conversation with analyst that performed tests. He suggested N_2 molecule was smaller than interstitial space of the 1-2mm fraction and was seeing "inside" the particles

Sarah Morris

From: Stan Morrison
Sent: Thursday, February 02, 2006 9:35 AM
To: Sarah Morris
Subject: FW: Micromeritics Analytical Services - Analysis Results

Sarah,

Surface Area results. I've included an Excel sheet ("Results_Surface Area") with the results tabulated (in the format your original data table). Of interest, the powdered sample was very similar to the coarser sample. Could you contact them and confirm that the samples were not powdered prior to analysis.

Thanks,

Stan
-----Original Message-----
From: michael.poston@micromeritics.com [mailto:michael.poston@micromeritics.com]
Sent: Thursday, February 02, 2006 7:49 AM
To: Stan Morrison
Cc: mark.talarico@micromeritics.com
Subject: Micromeritics Analytical Services - Analysis Results

CTO-01-08

Dear Stan Morrison,

Thank you for submitting your samples to Micromeritics Analytical Services. We appreciate the opportunity to serve you. Attached below, please find the results for your samples and a copy of the submission form (for future submissions). If you have any questions, comments or concerns please contact us at 770-662-3630.

Sincerely,

Michael Poston - Lab Analyst
Micromeritics Analytical Services
1 Micromeritics Dr.
Norcross, GA 30093
770.662.3630

www.particletesting.com

This e-mail is intended for the use of the addressee(s) only and may contain privileged, confidential, or proprietary information that is exempt from disclosure under law. If you have received this message in error, please inform us promptly by reply e-mail, then delete the e-mail and destroy any printed copy. Thank you.

Sarah Morris

From: Stan Morrison
nt: Thursday, February 02, 2006 1:02 PM
: Sarah Morris
ubject: RE: Micromeritics Info

Sarah,

Thanks. That satisfied my concern. Please put the response in the project file.

Stan

-----Original Message-----
From: Sarah Morris
Sent: Thursday, February 02, 2006 11:16 AM
To: Stan Morrison
Subject: Micromeritics Info

I just called and talked to the person that did the surface area analysis. He confirmed that the samples were analyzed as instructed, that the samples were not powdered prior.

When I told him your concern that the surface area of the 1-2 mm fraction was comparable to the powdered split, his response was that "it is possible that the N2 molecule was smaller than the interstitial space of the 1-2 mm fraction and was seeing "inside" the particles." He said that he was probably not the one to converse with about that possibility. If you wanted to call and discuss, the best person would be Greg Fields, their business manager who would probably be knowledgeable, but if he didn't, would know who to put you in contact with. Their number is 770-662-3630.

Sarah

CJD1-01-09

Crescent Junction Task 6 Kd

CJ01-01-10

2/9/2006 Prepare 2L SPF1. = Batch 1

2/10/2006 Spike soln ≅ 1mg/L U std. pH = 7.56

adjust pH to 6.57 ≅ 1.55mL conc HNO_3 U = 930.8ug/L cond = 27800 alk = 480

1000 add 100mL SPF1 ≅ U to the following then place on rotating bar @ 8RPM

	Mass	On	Off	SPF1 ≅ U	pH	Cond (uS/cm)	alk (mg/L)	U (ug/L)
CJ201@40	5g	2/10/06	2/11/06	Batch1	7.51	29400	650	898.0
201@40D	5g				7.53	29400	580	925.2
203@40	5				7.47	29400	560	892.2
204@40	5				7.49	29200	600	890.9
206@40	5				7.53	29400	540	906.1
207@40D	5				7.55	29400	610	823.9
208@40D	5				7.58	29400	570	831.4
209@40	5				7.50	29400	460	926.6
201@105	5				7.65	29500	640	850.1
202@105	5				7.65	29500	550	839.4
203@105	5				7.58	29400	610	821.2
204@105	5				7.61	29400	550	822.4
205@105	5				7.67	29400	560	839.3
205@105D	5				7.54	29500	570	820.2
206@105	5				7.52	29700	560	852.1
207@105	5				7.58	29700	610	798.0
208@105	5				7.57	29800	530	805.6
209@105	5				7.60	29600	600	813.6
210@105	5				7.56	29600	530	819.4
Batch1 Blank SPF1	0				7.46	29500	440	829.4

2/11/06 0930 Remove above from bar. Cent 20" x 300RPM. Filter thru 0.45um filter. Analyze

3

22-210

CJ01-01-11

CJ Task 6 Kd

2/12/06 0800 Check stability of SPF1=U, batch 2, start @ 4L, remaining 2L u = 942.3
pH = 6.88
add 0.6 mL conc HNO_3 pH = 6.58. Cond. = 29300 ORP = 217 alk = 640

place the following on rotating stir bar @ 8 RPM after adding 100 mL SPF1=U (Batch 2)

Sample	Mass	on	off	SPF1=U	pH	Cond (µS/cm)	Alk (mg/L as $CaCO_3$)	U (ug/L)
CJ207@40	10	2/12/06	2/13/06	Batch 2 day 2	7.59	28700	720	718.2
	20	↓	↓	↓	7.62	29000	690	704.6
	25				7.64	29200	720	704.4
CJ208@40	1				7.58	29200	650	775.4
	2				7.57	29000	680	747.3
	5				7.60	29000	680	753.6
	10				7.62	29100	720	753.7
	20				7.62	29100	730	729.4
	25				7.67	29200	710	734.2
CJ210@40	1				7.59	29300	630	766.8
	2				7.62	29200	760	751.7
	5				7.62	29100	650	757.6
	10				7.66	29100	700	732.4
	20				7.66	29100	780	705.8
	25				7.72	29100	750	735.4
SPF1=U Blank 3	∅	↓	↓	↓	7.50	29200	510	778.6

2/13/06 0745 Remove from stir bar. Cent 20" x 3500 RPM. Filter through 0.45 um filter. Analyze.

V

CJ01-01-12

Task 6 K1)

2/11/2006 1000 Place following on rotating stir bar @ 8 RPM after adding 100 mL SPFIEU (Batch 2 4L)

SPFIEU (Batch 2) = pH 6.63 alk = 690 mg/L as $CaCO_3$ U = 942.3 (mean) ng/L (measured 2/12/06 cond 29000 uS/cm)

Sample	Mins	on	off	SPFIEU	pH	Cond (uS/cm)	Alk (mg/L $CaCO_3$)	U (ug/L)
CJ202@40	1	2/11/06	2/12/06	Batch 2 day 1	7.47	29200	780	810.8
	2				7.51	29000	840	799.3
	5				7.52	29000	900	805.4
	10				7.53	28900	930	764.3
	20				7.53	28900	870	708.8
	25				7.58	28800	870	696.2
CJ205@40	1				7.53	28900	830	821.4
	2				7.54	29000	830	799.1
	5				7.54	28900	850	793.9
	10				7.56	29000	900	766.0
	20				7.58	28900	890	718.8
	25				7.60	28900	880	714.4
CJ207@40	1				7.54	29100	860	808.4
	2				7.50	29200	820	811.9
	5				7.48	29100	890	811.6
Blank SPFIEU Batch 2 Blank 2	Batch 2 day 1	Ø			7.39	29100	710	817.1

2/18/2006 Remove from stir bar Cent 20'' x 3000 RPM. Filter through 0.45 um filter. Analyze

(4)

Crescent Jctn. Task 6 Kd

CJ01-01-13

2/12/06 Prepare 1 L SPF2. Spike = 0.1 mL 10,000 mg/L. Concentration should measure 1000 ug/L U

Start pH = 7.84 adjust pH to 6.98 = 0.3 mL conc HNO_3 U = 893.9 ug/L
alk = 1000 cond = 22500 ORP = 203.9

2/13/06 Ck stability of SPF2 = U. pH ↑ 7.54. add 0.25 mL conc HNO_3 pH = 6.94
cond 22300 ORP 226.3 alk = 880 2/14/06 U = 765.0 ug/L (set overnight prior to analysis)

1PM add 100 mL SPF2 = U to the following

	Mass	on	off	SPF2 = U	pH	Cond (uS/cm)	Alk (mg/L as CaCO3)	U (ug/L)
CJ202@40	5g	2/13/06	2/14/06	Batch 1	7.59	22200	910	760.4
205@40	5				7.67	22400	880	765.0
207@40	5				7.76	22600	900	756.1
208@40	5				7.75	22700	900	789.5
208@40D	5				7.67	22600	930	752.1
210@40	5				7.69	24600	920	761.0
Blank 1 SPF2	0				7.55	24000	880	769.2

0930 Remove above from stir bar. Centrifuge 20" x 3500 RPM. Filter through 0.45 um filter analyze

2/21/2006 Prepare SPF3, will add U and pH adjust in AM

2/22/2006 SPF3 no U = 7.79 Add 0.11 mL 10K U (mg/L). Use 100 ul extra due to ↑ Vol of "1L recipe"

pH = 7.75, cond = 28200 uS/cm, ORP = 193.5 mV, alk = 280 mg/L as $CaCO_3$ U = 799.3 ug/L

0930 add 100 mL SPF3 = U to the following

(5)

22-210

Crescent Jctn. Task 6 Kd's

CJ01-01-14

2/22/06 SPF3 ≡ U 100mL to the following

0930

	Mass	On	Off	pH (end)	Cond us/cm (end)	Alk (end)	U (ug/L) end
CJ202@40	5g	2/22/06	2/23/06	7.88	28700	270	742.2
205@40	5			7.90	28900	270	756.7
207@40	5			7.91	28800	370	783.4
208@40	5			7.91	28700	270	797.0
210@40	5			7.93	29000	330	793.9
210@40D	5			7.92	28700	370	766.4
SPF3-	~~0~~			7.81	28600	250	~~867.8~~ 811.2 cm

2/23/06 0830 Remove from rotating stir bar. Centrifuge 3500RPM x 20" filter through 0.45μm filter analyze

Check SPF3 parent soln - day 2

pH = 7.75 Cond = 28500 ORP = 187.3 alk = 290 U = ~~818.1~~ 827.7 ug/L

SPF1

CJ01-01-15

	A	B	C	D	E	F	G	H	I	J	K	L
2			Solids									
3		mL per	mg per									
4		L of	L of	Na	K	Ca	Mg	NH4	SO4	Cl	NO3	C
5		Soln	Soln	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L
6	Liquid Components											
7	V2O5, V=998mg/L, 2%HNO3	0.00									0.00	
8	V2O5, V=1000mg/L, 5%HNO3	0.00									0.00	
9	**V2O5, V=1000mg/L, 1.4%HNO3**	0.00									0.00	
10	V2O5, V=1000mg/L, 2%HNO3	0.00									0.00	
11	Na2MoO4.2H2O, Mo=925mg/L	0.00		0.00								
12	Na2MoO4.2H2O, Mo=1000 mg/L,	0.00		0.00								
13	**(NH4)2MoO4, 1006 mg/L Mo**	0.00						0.00				
14	**U3O8, U=10000mg/L, 3.5%HNO3**	0.10									3.38	
15	U3O8, U=10000mg/L, 5.2%HNO3	0.00									0.00	
16	U Std, U=1000mg/L, 2% HNO3	0.00									0.00	
17	Ra Std, Ra=68.7pCi/mL, 2% HNO3	0.00									0.00	
18	As Std, As=999mg/L, 5%HNO3	0.00									0.00	
19	**As Std, As=1000mg/L, 1.4%HNO3**	0.00									0.00	
20	**Se =999 mg/L 5% HNO3**	0.00									0.00	
21	**Cd Std = 1000mg/L, ~2% HNO3**	0.00									0.00	
22												
23	100g/L K2CO3	0.00	0.00		0.00							0.00
24	10g/L KCl	0.00	0.00		0.00					0.00		
25	50g/L NaHCO3	38.00	1900.00	520.24								271.43
26	**100g/L Na2SO4.10H2O**	327.00	32700.00	4671.43					9749.07			
27	100g/L Na2SO4.(0.89 H2O)	0.00	0.00	0.00					0.00			
28	500g/L (NH4)2SO4	16.00	8000.00					2181.82	5818.18			
29	**1.5g/L CaSO4.2H2O**	600.00	900.00			209.62			502.09			
30	1.2 g/L CaSO4	0.00	0.00			0.00			0.00			
31	200g/L MgSO4.7H2O	16.00	3200.00				315.71		1247.26			
32	100g/L K2SO4	2.50	250.00		112.23				137.77			
33	conc H2SO4(36N)	0.00							0.00			
34	927.2 g/L CaCl2.2H2O	0.00	0.00			0.00				0.00		
35	92.72 g/L CaCl2.2H2O	0.00	0.00			0.00				0.00		
36	300g/L NaCl	5.00	1500.00	589.74						910.26		
37	100g/L MgCl2.6H2O	0.00	0.00				0.00			0.00		
38	100g/L NH4Cl	0.00	0.00					0.00		0.00		
39	100g/L NaNO3	0.00	0.00	0.00							0.00	
40	2% HNO3	0.00									0.00	
41	mL 1N NaOH needed to neutralize	0.00		0.00								
42	66.67 g/L NaN3	0.00	0.00	0.00								
43												
44												
45	Totals (mg/L)	1004.60		5781.41	112.23	209.62	315.71	2181.82	17454.37	910.26	3.38	271.43
46	ACTUAL (mg/L)			4674.00	108.00	207.00	303.00	2066	22076.00	1082.00	?	271.00
47	Totals (mol/L)			2.51E-01	2.87E-03	5.23E-03	1.30E-02	1.21E-01	1.82E-01	2.57E-02	5.46E-05	2.26E-02
48												
49	ACTUAL pH	6.63										
50	Measured pH(no acid or base)	?										
51	Measured pH (_____added)											
52	ACTUAL Alk (mg/L CaCO3)	1131.00										
53	Measured Alk (no acid or base)	?										
54	Measured Alk (_____added)											
55	EQ Acid per Liter	6.004E-05										
56												
57												

SPF2

CJ01-01-16

	A	B	C	D	E	F	G	H	I	J	K	L
2			Solids									
3		mL per	mg per									
4		L of	L of	Na	K	Ca	Mg	NH4	SO4	Cl	NO3	C
5		Soln	Soln	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L
6	Liquid Components											
7	V2O5, V=998mg/L, 2%HNO3	0.00									0.00	
8	V2O5, V=1000mg/L, 5%HNO3	0.00									0.00	
9	**V2O5, V=1000mg/L, 1.4%HNO3**	0.00									0.00	
10	V2O5, V=1000mg/L, 2%HNO3	0.00									0.00	
11	Na2MoO4.2H2O, Mo=925mg/L	0.00		0.00								
12	Na2MoO4.2H2O, Mo=1000 mg/L,	0.00		0.00								
13	**(NH4)2MoO4, 1006 mg/L Mo**	0.00						0.00				
14	**U3O8, U=10000mg/L, 3.5%HNO3**	0.00									0.00	
15	U3O8, U=10000mg/L, 5.2%HNO3	0.00									0.00	
16	U Std, U=1000mg/L, 2% HNO3	0.00									0.00	
17	Ra Std, Ra=68.7pCi/mL, 2% HNO3	0.00									0.00	
18	As Std, As=999mg/L, 5%HNO3	0.00									0.00	
19	**As Std, As=1000mg/L, 1.4%HNO3**	0.00									0.00	
20	**Se =999 mg/L 5% HNO3**	0.00									0.00	
21	**Cd Std = 1000mg/L, ~2% HNO3**	0.00									0.00	
22												
23	100g/L K2CO3	0.00	0.00		0.00							0.00
24	10g/L KCl	0.00	0.00		0.00					0.00		
25	50g/L NaHCO3	44.00	2200.00	602.38								314.29
26	**100g/L Na2SO4.10H2O**	356.00	35600.00	5085.71					10613.66			
27	100g/L Na2SO4.(0.89 H2O)	0.00	0.00	0.00					0.00			
28	500g/L (NH4)2SO4	7.60	3800.00					1036.36	2763.64			
29	**1.5g/L CaSO4.2H2O**	425.00	637.50			148.48			355.65			
30	1.2 g/L CaSO4	0.00	0.00			0.00			0.00			
31	200g/L MgSO4.7H2O	10.00	2000.00				197.32		779.54			
32	100g/L K2SO4	1.70	170.00		76.31				93.69			
33	conc H2SO4(36N)	0.00							0.00			
34	927.2 g/L CaCl2.2H2O	0.00	0.00			0.00				0.00		
35	92.72 g/L CaCl2.2H2O	0.00	0.00			0.00				0.00		
36	300g/L NaCl	1.70	510.00	200.51						309.49		
37	100g/L MgCl2.6H2O	0.00	0.00				0.00			0.00		
38	100g/L NH4Cl	0.00	0.00					0.00		0.00		
39	100g/L NaNO3	0.00	0.00	0.00							0.00	
40	2% HNO3	0.00									0.00	
41	mL 1N NaOH needed to neutralize	0.00		0.00								
42	66.67 g/L NaN3	0.00	0.00	0.00								
43												
44												
45	Totals (mg/L)	846.00		5888.61	76.31	148.48	197.32	1036.36	14606.17	309.49	0.00	314.29
46	ACTUAL (mg/L)			5887.00	74.00	148.00	191.00	1033	14888.00	315.00	?	315.00
47	Totals (mol/L)			2.56E-01	1.95E-03	3.70E-03	8.12E-03	5.76E-02	1.52E-01	8.73E-03	0.00E+00	2.62E-02
48												
49	ACTUAL pH	6.96										
50	Measured pH(no acid or base)	?										
51	Measured pH (_____added)											
52	ACTUAL Alk (mg/L CaCO3)	1497.00										
53	Measured Alk (no acid or base)	?										
54	Measured Alk (_____added)											
55	EQ Acid per Liter	0										
56												
57												

SPF3

	A	B	C	D	E	F	G	H	I	J	K	L
2			Solids									
3		mL per	mg per									
4		L of	L of	Na	K	Ca	Mg	NH4	SO4	Cl	NO3	C
5		Soln	Soln	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L
6	Liquid Components											
7	V2O5, V=998mg/L, 2%HNO3	0.00									0.00	
8	V2O5, V=1000mg/L, 5%HNO3	0.00									0.00	
9	**V2O5, V=1000mg/L, 1.4%HNO3**	0.00									0.00	
10	V2O5, V=1000mg/L, 2%HNO3	0.00									0.00	
11	Na2MoO4.2H2O, Mo=925mg/L	0.00		0.00								
12	Na2MoO4.2H2O, Mo=1000 mg/L,	0.00		0.00								
13	**(NH4)2MoO4, 1006 mg/L Mo**	0.00						0.00				
14	**U3O8, U=10000mg/L, 3.5%HNO3**	0.10									3.38	
15	U3O8, U=10000mg/L, 5.2%HNO3	0.00									0.00	
16	U Std, U=1000mg/L, 2% HNO3	0.00									0.00	
17	Ra Std, Ra=68.7pCi/mL, 2% HNO3	0.00									0.00	
18	As Std, As=999mg/L, 5%HNO3	0.00									0.00	
19	**As Std, As=1000mg/L, 1.4%HNO3**	0.00									0.00	
20	**Se =999 mg/L 5% HNO3**	0.00									0.00	
21	**Cd Std = 1000mg/L, ~2% HNO3**	0.00									0.00	
22												
23	100g/L K2CO3	0.00	0.00		0.00							0.00
24	10g/L KCl	0.00	0.00		0.00					0.00		
25	50g/L NaHCO3	11.00	550.00	150.60								78.57
26	**100g/L Na2SO4.10H2O**	474.00	47400.00	6771.43					14131.68			
27	100g/L Na2SO4.(0.89 H2O)	0.00	0.00	0.00					0.00			
28	500g/L (NH4)2SO4	6.60	3300.00					900.00	2400.00			
29	**1.5g/L CaSO4.2H2O**	560.00	840.00			195.65			468.62			
30	1.2 g/L CaSO4	0.00	0.00			0.00			0.00			
31	200g/L MgSO4.7H2O	9.10	1820.00				179.56		709.38			
32	100g/L K2SO4	3.70	370.00		166.10				203.90			
33	conc H2SO4(36N)	0.00							0.00			
34	927.2 g/L CaCl2.2H2O	0.00	0.00			0.00				0.00		
35	92.72 g/L CaCl2.2H2O	0.00	0.00			0.00				0.00		
36	300g/L NaCl	7.50	2250.00	884.62						1365.38		
37	100g/L MgCl2.6H2O	0.00	0.00				0.00			0.00		
38	100g/L NH4Cl	0.00	0.00					0.00		0.00		
39	100g/L NaNO3	0.00	0.00	0.00							0.00	
40	2% HNO3	0.00									0.00	
41	mL 1N NaOH needed to neutralize	0.00		0.00								
42	66.67 g/L NaN3	0.00	0.00	0.00								
43												
44												
45	Totals (mg/L)	1072.00		7806.64	166.10	195.65	179.56	900.00	17913.58	1365.38	3.38	78.57
46	ACTUAL (mg/L)			7800.00	166.00	196.00	180.00	900	19492.00	1336.00	?	79.20
47	Totals (mol/L)			3.40E-01	4.25E-03	4.88E-03	7.39E-03	5.00E-02	1.87E-01	3.85E-02	5.46E-05	6.55E-03
48												
49	ACTUAL pH	7.97										
50	Measured pH(no acid or base)	?										
51	Measured pH (_____added)											
52	ACTUAL Alk (mg/L CaCO3)	330.00										
53	Measured Alk (no acid or base)	?										
54	Measured Alk (_____added)											
55	EQ Acid per Liter	6.004E-05										
56												
57												

GQ1-01-17

Crescent Junction Task 7 Sequential Batch Leach CJ01-01-18

2/9/2006 Prepare 2L SPF1. PH adjust to 6.63. ē 0.9mL conc HNO_3

2/10/2006 Ck pH of SPF1. ↑ overnight to 7.34. add 0.6mL conc HNO_3 pH = 6.62 alk = 560 ORP = 197.4 cond 26800

9:00 Add 400mL pH adjusted SPF1 to following in 500mL Erlenmeyer flask

CJ-205-40 -2/+1 100g

CJ 203-40 -2/+1 100g

Place on orbital shaker table.

2/11/2006 0830. Remove from orbital shaker. Divide vol & solids between 2 ea 250ml / Nalge bottles per sample

Place in centrifuge @ 3500RPM x 20"

Decant and filter thru 0.45 um filter supernatant. Measure volume. Retain 50mL for analysis.

100g on orbital

CJ 205-205-2/+1 78.75 g in 315 mL residual SPF1 (365-50-315) 35mL in solids

CJ 204@40 -2/+1 78.75g in 315mL residual SPF1 (365-50=315) 35mL in solids

2/12/2006 0815 Remove from orbital shaker. Divide vol & solids between 2 ea 250ml Nalge
Place in centrifuge @ 3500RPM x 20"
Decant and filter thru 0.45 um filter. Vol = 290 mL both Retain 50mL for analysis
~25 mL retained in solids. (start 315 - 290 mL = 25mL retained in solids)

CJ 205@170 -2/+1 60 g in 240 mL residual SPF1

CJ 206@40 -2/+1 60 g in 240 mL residual SPF1

0900 Return to orbital shaker

(2)

CJ Task 7

CJ01-01-19

2/13/2006 0745 Remove from orbital shaker. Divide Vol & Solids between 2ea 250ml nalge
Place in centrifuge @3500RPM x 20"

Decant and filter through 0.45um filter. Vol = 215 ml (start 240-215ml = 25 ml retained in solids)
Horizontal test is complete. Retain all for analysis
Vertical test continues. Retain 50ml 205@176 for analysis

CJ205@235 -2/+1 4.25 g in 165 ml residual SPF1

Return to orbital shaker.

2/14/06 0900 Remove from orbital shaker. Divide vol & solids between 2ea 125ml nalge
Place in centrifuge @3500RPM x 20"

Decant and filter through 0.45um filter. Vol = 145 ml (start 165ml - 145 = 20 ml retained in solids)

Retain ~~46~~ 50ml CJ205@235 for analysis

CJ205@300 -2/+1 2.5 g in 100 ml residual SPF1

Return to orbital shaker

Measure SPF1 prep 2/9/06 pH, ORP, alk cond

2/15/05 0830 Remove from orbital shaker decant and filter thru 0.45um filter

Retain all for analysis

AMPAC EFFICIENCY LINE® 22-210

Crescent Jtn. Task 7 Sequential Batch Leach CJ01-01-20

Sample	1 Vol SPF1 mod (mL)	2 Mass (g)	3 pH	4 ORP (mV)	5 Cond (uS/cm)	6 Alk (mg/L as CaCO3)	7 Cl (mg/L)	8 NO3 (mg/L)	9 SO4 (mg/L)	10 NH3-N (mg/L)	11 U (ug/L)	12	13
CJ203@40	400	100	7.66	196.7	29400	560	1026	764	18676	1700	5.5	note - samples are yellow tinged	
204@40	315	78.75	7.79	186.3	30100	450	1096	828	19872	1500	19.3		
206@40	240	60	7.83	175.2	29900	560	1120	820	19910	1300	25.4		
CJ 205@40	400	100	7.73	187.3	29200	620	1106	756	18504	1600	3.0		
@105	315	78.75	7.85	171.4	29800	560	1116	770	18828	1400	19.5		
@170	240	60	7.96	171.5	29600	520	1196	776	19032	1100	29.0		
@235	165	41.25	7.85	173.3	29700	400	1284	804	19700	1800	44.9		
@300	100	25	7.97	173.5	30600	330	1336	794	19492	900	54.5		
Start Dolw SPF1 mod	9/10	~~0~~ 8	6.62	197.4	26800	560	~~1018~~	~~738~~	~~18272~~	2000	<0.1		
SPF1 mod	9/14		7.85	191.9	29600	510	1018	738	18272	2000			

Crescent Jctn. Task 7 Sequential Batch Leach (Data Cont) CJ01-01-21

Sample	[1] Vol SPFL mL (mL)	[2] Mass (g)	[3] #	[4] Ca (mg/L)	[5] Na (mg/L)	[6] Mg (mg/L)	[7] K (mg/L)	8	9	10	11	12	13
CJ203e40	400	100		320	5100	440	141						
204e40	315	78.75		350	5400	510	156						
206e40	240	60		349	6300	300	177						
CJ205e40	400	100		236	5700	210	141						
e105	315	78.75		220	6400	200	168						
e170	240	60		199	6500	250	157						
e235	165	41.25		203	7000	180	167						
e300	100	25		196	7800	180	166						
SPFL				196	5300	310	129						

Appendix C

Complete Chemical Results and Computations

(1) Loss on Drying
(2) Size Fraction Analysis
(3) X-Ray Diffraction Results
(4) Surface Area Results
(5) Cation Exchange Capacity Results
(6) Water Soluble Minerals – Raw Data
(7) Water Soluble Minerals – NETPATH Results
(8) Water Soluble Minerals – PHREEQC Input
(9) Distribution Ratios: Single-Point, SPF1
(10) Distribution Ratios: Single-Point, SPF2
(11) Distribution Ratios: Single-Point, SPF3
(12) Distribution Ratios: Multiple-Point Isotherms
(13) Results of Sequential Batch Tests

S.M.Stoller

Point of Contact:

Sarah Morris

248-6514

Crescent Junction Core Analysis

01/09/06

Instructions to Geotech Engineering Group for sample prep:

DO NOT PULVERIZE

Gently disaggregate samples to -10/+18 (1 to 2 mm nominal diameter)

Avoid (as much as possible) generating heat.

Some samples still have a moderate water content.

Once disaggregated, place in labeled, sealed ziplock bags to avoid loosing moisture content.

Note: Unless noted in comments column, an ~2 inch sample was obtained starting at the even depth indicated

Sample	Tare	Gross Wet	Gross Dry	Net Wet	Net Dry	LOD (g)	LOD (%)	Comments
CJ-201-40	6.7	352.2	342.5	345.5	335.8	9.7	2.81%	
CJ-201-105	6.7	382.4	377.6	375.7	370.9	4.8	1.28%	
CJ-201-170	6.7	322.7	317.6	316	310.9	5.1	1.61%	169'10"
CJ-201-235	6.7	360.5	355.9	353.8	349.2	4.6	1.30%	
CJ-201-300	6.7	366.7	360.8	360	354.1	5.9	1.64%	
CJ-202-40	6.7	348.6	338.3	341.9	331.6	10.3	3.01%	
CJ-202-105	6.7	344.9	339	338.2	332.3	5.9	1.74%	
CJ-202-170	6.7	250.6	244.7	243.9	238	5.9	2.42%	
CJ-202-235	6.7	358.3	353.7	351.6	347	4.6	1.31%	
CJ-202-300	6.7	301.8	297.9	295.1	291.2	3.9	1.32%	299'10"
CJ-203-40	6.7	395.8	386.8	389.1	380.1	9	2.31%	
CJ-203-105	6.7	447.3	440.7	440.6	434	6.6	1.50%	
CJ-203-170	6.7	445.9	438.4	439.2	431.7	7.5	1.71%	
CJ-203-235	6.7	368.5	362.6	361.8	355.9	5.9	1.63%	
CJ-203-300	6.7	438.1	431.3	431.4	424.6	6.8	1.58%	
CJ-204-40	6.7	350.3	340.7	343.6	334	9.6	2.79%	
CJ-204-105	6.7	309.1	303.2	302.4	296.5	5.9	1.95%	
CJ-204-170	6.7	395.8	389.2	389.1	382.5	6.6	1.70%	
CJ-204-235	6.7	306.1	301.3	299.4	294.6	4.8	1.60%	
CJ-204-300	6.7	410.9	404.9	404.2	398.2	6	1.48%	
CJ-205-40	6.7	631	621.3	624.3	614.6	9.7	1.55%	Obtain addt'l sample
CJ-205-105	6.7	378.3	371.2	371.6	364.5	7.1	1.91%	
CJ-205-170	6.7	414.8	408.4	408.1	401.7	6.4	1.57%	
CJ-205-235	6.7	324.7	318.5	318	311.8	6.2	1.95%	234'10"
CJ-205-300	6.7	396.3	390.9	389.6	384.2	5.4	1.39%	299'10"
CJ-206-40	6.7	427.7	420.1	421	413.4	7.6	1.81%	
CJ-206-105	6.7	465.6	458.1	458.9	451.4	7.5	1.63%	
CJ-206-170	6.7	401.8	395.6	395.1	388.9	6.2	1.57%	
CJ-206-235	6.7	311	305.4	304.3	298.7	5.6	1.84%	
CJ-206-300	6.7	456	449.8	449.3	443.1	6.2	1.38%	
CJ-207-40	6.7	414	407	407.3	400.3	7	1.72%	
CJ-207-105	6.7	380.6	374.2	373.9	367.5	6.4	1.71%	
CJ-207-170	6.7	354.4	349.4	347.7	342.7	5	1.44%	
CJ-207-235	6.7	376.6	371.3	369.9	364.6	5.3	1.43%	
CJ-207-300	6.7	384.8	379.6	378.1	372.9	5.2	1.38%	299'10"
CJ-208-40	6.7	387.4	384.5	380.7	377.8	2.9	0.76%	39'10"
CJ-208-105	6.7	364.2	360.1	357.5	353.4	4.1	1.15%	
CJ-208-170	6.7	445.4	437.8	438.7	431.1	7.6	1.73%	169'10"
CJ-208-235	6.7	393.5	387.6	386.8	380.9	5.9	1.53%	
CJ-208-300	6.7	394.2	389.8	387.5	383.1	4.4	1.14%	
CJ-209-40	6.7	320.4	314.5	313.7	307.8	5.9	1.88%	
CJ-209-105	6.7	392.8	387	386.1	380.3	5.8	1.50%	
CJ-209-170	6.7	475.7	470.2	469	463.5	5.5	1.17%	

Sample	Tare	Gross	Gross	Net Wet	Net Dry	LOD	LOD	Comments			
		Wet	Dry			(g)	(%)				
CJ-209-235	6.7	390.1	385.3	383.4	378.6	4.8	1.25%				
CJ-209-300	6.7	521.4	516.6	514.7	509.9	4.8	0.93%	299'10"			
CJ-210-40	6.7	376.6	369.9	369.9	363.2	6.7	1.81%				
CJ-210-105	6.7	299	296.2	292.3	289.5	2.8	0.96%				
CJ-210-170	6.7	391.1	386.1	384.4	379.4	5	1.30%				
CJ-210-235	6.7	392.1	386.3	385.4	379.6	5.8	1.50%				
CJ-210-300	6.7	415.1	409.6	408.4	402.9	5.5	1.35%				

S.M.Stoller

Point of Contact:

Sarah Morris

248-6514

Crescent Junction Core Analysis

01/09/06

Samples returned from Geotech Engineering Group

Disaggregated prior to LOD, some samples powdered easily, so greater >1mm fraction than anticipated

Splits are function of mild disaggregation, not indicative of true particle size

Air Dried, Sieved

+10 mesh = >2mm

-10/+18 = 1-2mm

-18 = <1mm

Sample	Net Total Mass	+2mm gross (g)	+2mm (g)	+2mm (%)	1-2mm gross (g)	1-2mm (g)	1-2mm (%)	<1mm gross (g)	<1mm (g)	<1mm (%)		Frac >1 (g)
CJ-201-40	335.8	21.3	14.6	4.35%	147.8	141.1	42.02%	184.6	177.9	52.98%	99.34%	155.7
CJ-201-105	370.9	23.8	17.1	4.61%	159.1	152.4	41.09%	206.8	200.1	53.95%	99.65%	169.5
CJ-201-170	310.9	38.5	31.8	10.23%	131.5	124.8	40.14%	159.4	152.7	49.12%	99.49%	156.6
CJ-201-235	349.2	103.3	96.6	27.66%	112.7	106	30.36%	151.6	144.9	41.49%	99.51%	202.6
CJ-201-300	354.1	101	94.3	26.63%	122.9	116.2	32.82%	148.7	142	40.10%	99.55%	210.5
CJ-202-40	331.6	93	86.3	26.03%	104.8	98.1	29.58%	152.5	145.8	43.97%	99.58%	184.4
CJ-202-105	332.3	102.4	95.7	28.80%	102.6	95.9	28.86%	146.3	139.6	42.01%	99.67%	191.6
CJ-202-170	238	71.9	65.2	27.39%	85.9	79.2	33.28%	98.7	92	38.66%	99.33%	144.4
CJ-202-235	347	90.5	83.8	24.15%	119	112.3	32.36%	156.4	149.7	43.14%	99.65%	196.1
CJ-202-300	291.2	95.5	88.8	30.49%	97.2	90.5	31.08%	116.3	109.6	37.64%	99.21%	179.3
CJ-203-40	380.1	68.3	61.6	16.21%	120.8	114.1	30.02%	210.1	203.4	53.51%	99.74%	175.7
CJ-203-105	434	110.4	103.7	23.89%	138.2	131.5	30.30%	203.8	197.1	45.41%	99.61%	235.2
CJ-203-170	431.7	152.1	145.4	33.68%	138.5	131.8	30.53%	159.3	152.6	35.35%	99.56%	277.2
CJ-203-235	361.8	151.1	144.4	39.91%	99.4	92.7	25.62%	124.3	117.6	32.50%	98.04%	237.1
CJ-203-300	431.4	155	148.3	34.38%	118.7	112	25.96%	168.3	161.6	37.46%	97.80%	260.3
CJ-204-40	343.6	100.8	94.1	27.39%	90.8	84.1	24.48%	160.7	154	44.82%	96.68%	178.2
CJ-204-105	302.4	122.7	116	38.36%	79.7	73	24.14%	112.7	106	35.05%	97.55%	189
CJ-204-170	389.1	188.9	182.2	46.83%	90.4	83.7	21.51%	122	115.3	29.63%	97.97%	265.9
CJ-204-235	299.4	124.7	118	39.41%	78.4	71.7	23.95%	109.5	102.8	34.34%	97.70%	189.7
CJ-204-300	404.2	175.4	168.7	41.74%	113	106.3	26.30%	128.1	121.4	30.03%	98.07%	275
CJ-205-40	624.3	171.3	164.6	26.37%	186.6	179.9	28.82%	274.2	267.5	42.85%	98.03%	344.5
CJ-205-105	371.6	116	109.3	29.41%	123.2	116.5	31.35%	144	137.3	36.95%	97.71%	225.8
CJ-205-170	408.1	120.2	113.5	27.81%	135.8	129.1	31.63%	163.6	156.9	38.45%	97.89%	242.6
CJ-205-235	318	120.8	114.1	35.88%	97.4	90.7	28.52%	112	105.3	33.11%	97.52%	204.8
CJ-205-300	389.6	147.8	141.1	36.22%	112.9	106.2	27.26%	142.2	135.5	34.78%	98.25%	247.3
CJ-206-40	421	154	147.3	34.99%	104.9	98.2	23.33%	172.1	165.4	39.29%	97.60%	245.5
CJ-206-105	458.9	148.1	141.4	30.81%	130.5	123.8	26.98%	191.2	184.5	40.20%	98.00%	265.2
CJ-206-170	395.1	153	146.3	37.03%	121.7	115	29.11%	133.1	126.4	31.99%	98.13%	261.3
CJ-206-235	304.3	100.8	94.1	30.92%	101.3	94.6	31.09%	115.7	109	35.82%	97.83%	188.7
CJ-206-300	449.3	181.6	174.9	38.93%	129	122.3	27.22%	150.6	143.9	32.03%	98.17%	297.2
CJ-207-40	407.3	161.3	154.6	37.96%	108.6	101.9	25.02%	149.8	143.1	35.13%	98.11%	256.5
CJ-207-105	373.9	154.4	147.7	39.50%	100.2	93.5	25.01%	131.1	124.4	33.27%	97.78%	241.2
CJ-207-170	347.7	145.6	138.9	39.95%	96.8	90.1	25.91%	119.6	112.9	32.47%	98.33%	229
CJ-207-235	369.9	140.6	133.9	36.20%	117	110.3	29.82%	125.7	119	32.17%	98.19%	244.2
CJ-207-300	378.1	119.3	112.6	29.78%	135.5	128.8	34.07%	136.4	129.7	34.30%	98.15%	241.4
CJ-208-40	380.7	106.7	100	26.27%	114.8	108.1	28.40%	175.1	168.4	44.23%	98.90%	208.1
CJ-208-105	357.5	107	100.3	28.06%	112.5	105.8	29.59%	151.9	145.2	40.62%	98.27%	206.1
CJ-208-170	438.7	164	157.3	35.86%	139.7	133	30.32%	146.1	139.4	31.78%	97.95%	290.3
CJ-208-235	386.8	142.7	136	35.16%	122.7	116	29.99%	133.9	127.2	32.89%	98.04%	252
CJ-208-300	387.5	72.6	65.9	17.01%	146.2	139.5	36.00%	182.6	175.9	45.39%	98.40%	205.4
CJ-209-40	313.7	65.6	58.9	18.78%	107.5	100.8	32.13%	152.5	145.8	46.48%	97.39%	159.7

Sample	Net Total	+2mm	+2mm	+2mm	1-2mm	1-2mm	1-2mm	<1mm	<1mm	<1mm		Frac >1
	Mass	gross (g)	(g)	(%)	gross (g)	(g)	(%)	gross (g)	(g)	(%)		(g)
CJ-209-105	386.1	123.7	117	30.30%	130.3	123.6	32.01%	145.1	138.4	35.85%	98.16%	240.6
CJ-209-170	469	89.4	82.7	17.63%	169.9	163.2	34.80%	222.2	215.5	45.95%	98.38%	245.9
CJ-209-235	383.4	95.3	88.6	23.11%	135.6	128.9	33.62%	166.5	159.8	41.68%	98.41%	217.5
CJ-209-300	514.7	100.2	93.5	18.17%	198.9	192.2	37.34%	227.8	221.1	42.96%	98.47%	285.7
CJ-210-40	369.9	128.4	121.7	32.90%	115.3	108.6	29.36%	138.1	131.4	35.52%	97.78%	230.3
CJ-210-105	292.4	65.3	58.6	20.04%	102	95.3	32.59%	141	134.3	45.93%	98.56%	153.9
CJ-210-170	384.4	98.4	91.7	23.86%	139.3	132.6	34.50%	159.7	153	39.80%	98.15%	224.3
CJ-210-235	385.4	110.7	104	26.98%	140.1	133.4	34.61%	147.3	140.6	36.48%	98.08%	237.4
CJ-210-300	408.4	96.2	89.5	21.91%	153.4	146.7	35.92%	171.8	165.1	40.43%	98.26%	236.2

XRD Analysis

Bill Hood

SM Stoller

Point of Contact: Stan Morrison 248-6373

Dr. Hood received 1/17/2006

Samples sent to Bill are <1mm fraction

Bill Hood provided a report to Stan on February 6, 2006

Summary: (1) non-phyllosilicate minerals identified include quartz, calcite, dolomite, orthoclase, plagioclase, and gysum (2) Clay minerals (in order of abundance) include: mixed-layer illite smectite (at least 60% illite layers), discrete illite, kaolinite, and mixed-layer chlorite-vermiculite.

Samples	*Estimated Abundances (%) of Non-Phyllosilicates in Bulk Samples*					
	Quartz	Calcite	Dolomite	Orthoclase	Plagioclase	Gypsum
CJ-201-40	32	3	5	1	1	Tr
CJ-202-40	29	3	4	1	1	1
CJ-203-40	36	4	5	1	2	1
CJ-204-40	33	2	3	1	1	
CJ-205-40	28	3	6	1	1	
CJ-206-40	39	4	6	1	2	
CJ-207-40	25	3	3	1	1	
CJ-208-40	38	3	5	1	1	
CJ-209-40	27	1	3	2	1	Tr
CJ-210-40	24	4	3	1	1	

Samples	*Estmated Abundances (%) of Clays*				I/S
	Mixed-Layer	Illite	Kaolinite		%Illite
CJ-201-40	43	29	28		70
CJ-202-40	38	36	26		60
CJ-203-40	43	31	25		60
CJ-204-40	40	30	29		60
CJ-205-40	46	31	23		60
CJ-206-40	37	34	29		60
CJ-207-40	27	36	37		50
CJ-208-40	35	36	29		60
CJ-209-40	39	31	29		60
CJ-210-40	39	37	25		60

Micromeritics Analytical Services			
One Micromeritics Drive			
Norcross, GA 30093-1877			
1-770-662-3630			
Multi-point Surface Area Analysis, BET Method			
Catalog #005-01			
Sample	Particle	Surface	
	size	Area	
		m2/g	
CJ-201-40	1 to 2 mm	10.6561	
CJ-202-40	1 to 2 mm	12.2117	
CJ-203-40	1 to 2 mm	8.8087	
CJ-204-40	1 to 2 mm	12.9162	
CJ-205-40	1 to 2 mm	9.9511	
CJ-206-40	1 to 2 mm	9.4615	
CJ-207-40	1 to 2 mm	13.1245	
CJ-208-40	1 to 2 mm	9.3897	
CJ-209-40	1 to 2 mm	10.456	
CJ-210-40	1 to 2 mm	13.2247	
	Mean =	11.02002	
	min =	8.8087	
	max =	13.2247	
CJ-205-40-P	<1 mm	10.6955	

Cation Exchange Capacity			
Samples	Size	NH3-N	CEC
		(mg/L)	(meq/100g)
CJ-201-40	1-2 mm	0.65	9.29
CJ-202-40	1-2 mm	0.82	11.71
CJ-203-40	1-2 mm	2.54	36.29
CJ-204-40	1-2 mm	0.75	10.71
CJ-205-40	1-2 mm	0.75	10.71
CJ-205-40-Dup	1-2 mm	0.89	12.71
CJ-205-40-P	<1 mm	0.72	10.29
CJ-205-40-P-Dup	<1 mm	0.73	10.43
CJ-206-40	1-2 mm	0.41	5.86
CJ-207-40	1-2 mm	1.08	15.43
CJ-208-40	1-2 mm	0.49	7.00
CJ-209-40	1-2 mm	1.19	17.00
CJ-210-40	1-2 mm	0.8	11.43
CJ-201-105	1-2 mm	0.37	5.29
CJ-202-105	1-2 mm	0.8	11.43
CJ-203-105	1-2 mm	0.49	7.00
CJ-204-105	1-2 mm	0.9	12.86
CJ-204-105-Dup	1-2 mm	0.92	13.14
CJ-205-105	1-2 mm	0.87	12.43
CJ-206-105	1-2 mm	0.52	7.43
CJ-207-105	1-2 mm	0.6	8.57
CJ-208-105	1-2 mm	0.5	7.14
CJ-209-105	1-2 mm	1.03	14.71
CJ-210-104	1-2 mm	0.038	0.54
	min=	0.04	0.54
	Max =	2.54	36.29
	Mean	0.79	11.23

Water Soluble Fractions: Used 2 g of sample leached with 100 mL of deionized water														
Sample	Depth	pH	Cond	ORP	Alk	Cl	NO3-N	SO4	U	NH3-N	Ca	Na	Mg	K
	ft		(uS/cm)	(mV)	(mg/L as	(mg/L)	(mg/L)	(mg/L)	(ug/L)	(mg/L)	(mg/L)	(mg/L)	(mg/L)	(mg/L)
CJ-201-40	40	7.97	258	136	9	7.98	0.22	79.28	0.27	0.11	13.9	20.8	3.4	9.7
CJ-201-105	105	9.39	147	104	39	6.88	**0.11**	7.33	0.95	0.08	0.76	24	0.16	2.8
CJ-201-170	170	9.78	212	95	77	7.16	**0.11**	4.98	1.29	0.3	0.15	36.5	0.12	4.4
CJ-201-235	235	9.81	220	87	82	6.75	**0.11**	3.36	1.42	0.4	0.1	38.5	0.11	4.4
CJ-201-300	300	9.86	254	98	93	8.24	**0.11**	3.61	1.47	0.41	0.09	43	0.11	6.6
CJ-202-40	40	9.26	170	113	36	9.88	0.51	16.32	1.01	0.12	0.45	20	0.76	15.1
CJ-202-40-D	40	9.12	135	56	38	4.25	0.49	16.18	0.36	0.09	0.48	20.5	0.81	3.6
CJ-202-105	105	9.78	267	116	83	17.37	**0.11**	4.32	0.81	0.33	0.18	36	0.12	17.2
CJ-202-170	170	9.79	238	99	89	4.51	**0.11**	5.38	10.37	0.43	0.11	41	0.1	3.5
CJ-202-235	235	9.8	214	88	81	6.12	**0.11**	4.47	0.87	0.33	0.12	36	0.1	3.2
CJ-202-300	300	9.81	251	105	86	11.11	**0.11**	3.96	0.81	0.32	0.17	38	0.08	10.8
CJ-203-40	40	6.17	800	89	12	3.18	0.30	412.9	0.19	0.2	122.4	9	8	2
CJ-203-105	105	9.52	217	113	49	17.73	**0.11**	7.54	0.69	0.26	0.45	29	0.13	16.3
CJ-203-170	170	9.75	207	96	76	6.9	**0.11**	5.53	1.11	0.28	0.22	36	0.13	3.3
CJ-203-235	235	9.8	237	92	89	6.67	**0.11**	5.9	1.11	0.51	0.08	41	0.1	4.8
CJ-203-300	300	9.7	201	85	76	6.95	**0.11**	3.78	0.82	0.38	0.11	36	0.1	3.2
CJ-204-40	40	7.81	431	85	15	2.74	**0.11**	171.05	0.23	0.42	36.8	26	7	2.12
CJ-204-40-D	40	8.46	383	65	19	2.69	**0.11**	146.47	0.20	0.41	30.4	27	6.2	2.2
CJ-204-105	105	9.85	232	84	87	5.22	**0.11**	5.09	1.32	0.35	0.1	40	0.11	5.6
CJ-204-170	170	9.81	221	84	83	8.03	**0.11**	5.29	1.02	0.48	0.09	37	0.11	4.6
CJ-204-235	235	9.74	193	84	65	7.56	**0.11**	6.03	0.69	0.47	0.18	32	0.09	3.3
CJ-204-300	300	9.85	232	79	91	5.4	**0.11**	4.34	0.94	0.44	0.03	40	0.1	3.2
CJ-205-40	40	9.16	146	97	37	4.62	**0.11**	15.71	0.72	0.4	0.25	24.5	0.37	6.5
CJ-205-105	105	9.73	247	95	93	7.38	**0.11**	6.6	1.13	0.47	0.06	41	0.12	4.6
CJ-205-170	170	9.68	246	85	96	6.03	**0.11**	5.49	1.07	0.47	0.07	42	0.1	4.7
CJ-205-235	235	9.67	257	84	90	5.19	**0.11**	9.04	1.24	0.54	0.11	44	0.09	2.6
CJ-205-300	300	9.73	224	78	85	5.17	**0.11**	5.87	0.81	0.46	0.13	38	0.08	2.5
CJ-206-40	40	8.78	143	77	35	5.18	**0.11**	22.23	0.21	0.23	1.25	21.5	0.72	2.3
CJ-206-40-D	40	9.07	144	62	29	5.02	**0.11**	21.28	0.17	0.25	1.37	21.5	0.76	2.2
CJ-206-105	105	9.29	153	76	44	6.45	**0.11**	8.59	0.26	0.29	0.69	23	0.79	2.2
CJ-206-170	170	9.76	237	75	92	6.31	**0.11**	4.47	1.04	0.44	0.1	39	0.1	3
CJ-206-235	235	9.71	219	74	84	6.73	**0.11**	5.05	0.65	0.52	0.12	37	0.09	2.9
CJ-206-300	300	9.63	214	72	86	6.66	**0.11**	2.07	0.52	0.41	0.12	37	0.09	2.5
CJ-207-40	40	9.64	273	75	81	4.2	**0.11**	29.84	1.53	0.72	0.09	50	0.14	4.8
CJ-207-105	105	9.61	171	68	68	5.48	**0.11**	4.31	0.47	0.3	0.29	27	0.11	2.3
CJ-207-170	170	9.63	201	71	76	5.79	**0.11**	5.53	0.61	0.46	0.16	33	0.11	3
CJ-207-235	235	9.75	241	71	91	5.42	**0.11**	5.38	0.80	0.48	0.11	40	0.08	2.5
CJ-207-300	300	9.76	247	70	94	5.04	**0.11**	5.84	0.81	0.46	0.08	41	0.07	2.5
CJ-208-40	40	9.29	138	69	32	6.44	**0.11**	16.71	0.20	0.15	1.05	21	0.38	1.6
CJ-208-40-D	40	9.27	134	80	35	5.97	**0.11**	16.63	0.16	0.2	1.42	27.5	0.46	1.8
CJ-208-105	105	9.31	156	71	39	6.61	**0.11**	11.62	0.26	0.25	0.69	24	0.19	2.1
CJ-208-170	170	9.8	261	71	101	6.04	**0.11**	5.74	0.15	0.38	0.08	44	0.09	3.3
CJ-208-235	235	9.81	251	69	97	5.51	**0.11**	4.25	0.87	0.51	0.07	42	0.08	2.9
CJ-208-300	300	9.64	192	66	72	6.47	**0.11**	4.71	0.34	0.35	0.23	31	0.08	2
CJ-209-40	40	8.49	254	89	20	2.47	**0.11**	81.97	0.12	**0.08**	5	31	3.6	3.9
CJ-209-105	105	9.77	250	75	93	5.1	**0.11**	7.43	0.95	0.42	0.14	43	0.11	2.9
CJ-209-170	170	9.51	179	72	59	6.87	**0.11**	6.67	0.25	0.37	0.33	35	0.12	2.4
CJ-209-235	235	9.78	226	72	88	6.07	**0.11**	5.94	0.45	0.34	0.13	38	0.08	2.4
CJ-209-300	300	9.88	254	66	104	5.05	**0.11**	3.45	0.81	0.6	0.08	43	0.08	2.2
CJ-210-40	40	9.72	221	63	73	4.99	**0.11**	15.6	0.75	0.33	0.19	38	0.13	3.1
CJ-210-105	105	9.32	138	59	39	7.11	**0.11**	9.56	0.14	0.2	1.02	20	0.23	1.9
CJ-210-170	170	9.77	212	60	79	6.31	**0.11**	5.65	0.72	0.41	0.17	36	0.09	2.3
CJ-210-235	235	9.81	230	59	90	6.04	**0.11**	4.57	0.67	0.38	0.1	39	0.07	2.3
CJ-210-300	300	9.83	249	58	99	5.5	**0.11**	5.12	0.76	0.41	0.09	43	0.07	2.2

Water Soluble Fraction Results from NETPATH output files										
Sample	**Depth**	**pH**	**Calcite**	**Gypsum**	**Nahcolite**	**Halite**	**Sylvite**	**Exchange**	**Dolomite**	**Total**
			CaCO3	**CaSO4**	**NaHCO3**	**NaCl**	**KCl**	**Ca/Na**	**CaMg(CO3)2**	
			mmol/L	**mmol/L**	**mmol/L**	**mmol/L**	**mmol/L**	**mmol/L**	**mmol/L**	**mmol/L**
CJ-201-40	40	7.97	-0.21	0.82	0.11	-0.02	0.25	0.41	0.14	1.50
CJ-202-40	40	9.26	0.02	0.17	0.55	-0.11	0.39	0.21	0.03	1.26
CJ-203-40	40	6.17	-2.70	4.30	2.60	0.04	0.05	-1.12	0.33	3.50
CJ-204-40	40	7.81	-0.92	1.78	0.65	0.02	0.05	0.23	0.29	2.10
CJ-205-40	40	9.16	0.12	0.16	0.51	-0.04	0.17	0.30	0.02	1.24
CJ-206-40	40	8.78	-0.22	0.23	0.83	0.09	0.06	0.01	0.03	1.03
CJ-207-40	40	9.64	0.28	0.31	0.99	**-0.01**	0.12	0.60	0.01	2.30
CJ-208-40	40	9.29	-0.08	0.17	0.61	0.14	0.04	0.08	0.02	0.98
CJ-209-40	40	8.49	-0.46	0.85	0.56	-0.03	0.10	0.41	0.15	1.58
CJ-210-40	40	9.72	0.15	0.16	0.97	0.06	0.08	0.31	**0.01**	1.74
CJ-201-105	105	9.39	0.14	0.08	0.52	0.12	0.07	0.20	0.01	1.14
CJ-202-105	105	9.78	0.18	0.04	1.07	0.05	0.44	0.22	**0.01**	2.01
CJ-203-105	105	9.52	0.24	0.08	0.56	0.08	0.42	0.31	0.01	1.70
CJ-204-105	105	9.85	0.36	0.05	0.91	**0.01**	0.14	0.41	**0.01**	1.89
CJ-205-105	105	9.73	0.12	0.07	1.31	0.09	0.12	0.19	**0.01**	1.91
CJ-206-105	105	9.29	-0.04	0.09	0.75	0.12	0.06	0.06	0.03	1.07
CJ-207-105	105	9.61	-0.10	0.04	1.19	0.10	0.06	-0.05	**0.01**	1.25
CJ-208-105	105	9.31	0.02	0.12	0.64	0.13	0.05	0.13	0.01	1.10
CJ-209-105	105	9.77	0.23	0.08	1.17	0.07	0.07	0.31	**0.01**	1.94
CJ-210-105	105	9.32	-0.11	0.10	0.77	0.15	0.05	-0.03	0.01	0.94
CJ-201-170	170	9.78	0.24	0.05	0.92	0.09	0.11	0.29	**0.01**	1.71
CJ-202-170	170	9.79	0.30	0.06	1.04	0.04	0.09	0.35	**0.01**	1.89
CJ-203-170	170	9.75	0.19	0.06	0.97	0.11	0.08	0.24	0.01	1.66
CJ-204-170	170	9.81	0.16	0.06	1.07	0.11	0.12	0.22	**0.01**	1.75
CJ-205-170	170	9.68	0.14	0.06	1.37	0.05	0.12	0.21	**0.01**	1.96
CJ-206-170	170	9.76	0.10	0.05	1.30	0.10	0.08	0.15	**0.01**	1.79
CJ-207-170	170	9.63	0.02	0.06	1.19	0.09	0.08	0.08	**0.01**	1.53
CJ-208-170	170	9.80	0.18	0.06	1.33	0.09	0.08	0.25	**0.01**	2.00
CJ-209-170	170	9.51	0.28	0.07	0.68	0.13	0.06	0.35	**0.01**	1.58
CJ-210-170	170	9.77	0.14	0.06	1.05	0.12	0.06	0.20	**0.01**	1.64
CJ-201-235	235	9.81	0.31	0.03	0.91	0.08	0.11	0.35	**0.01**	1.80
CJ-202-235	235	9.80	0.17	0.05	1.04	0.09	0.08	0.22	**0.01**	1.66
CJ-203-235	235	9.80	0.27	0.06	1.06	0.06	0.12	0.33	**0.01**	1.91
CJ-204-235	235	9.74	0.16	0.06	0.82	0.13	0.08	0.22	**0.01**	1.48
CJ-205-235	235	9.67	0.23	0.09	1.19	0.08	0.07	0.32	**0.01**	1.99
CJ-206-235	235	9.71	0.09	0.05	1.21	0.12	0.07	0.14	**0.01**	1.69
CJ-207-235	235	9.75	0.14	0.06	1.24	0.09	0.06	0.20	**0.01**	1.80
CJ-208-235	235	9.81	0.21	0.04	1.24	0.08	0.07	0.25	**0.01**	1.90
CJ-209-235	235	9.78	0.09	0.06	1.24	0.11	0.06	0.15	**0.01**	1.72
CJ-210-235	235	9.81	0.15	0.05	1.20	0.11	0.06	0.19	**0.01**	1.77
CJ-201-300	300	9.86	0.37	0.04	0.98	0.06	0.17	0.41	**0.01**	2.04
CJ-202-300	300	9.81	0.25	0.04	1.03	0.04	0.28	0.29	**0.01**	1.94
CJ-203-300	300	9.70	0.19	0.04	0.98	0.11	0.08	0.23	**0.01**	1.64
CJ-204-300	300	9.85	0.24	0.05	1.09	0.07	0.08	0.29	**0.01**	1.83
CJ-205-300	300	9.73	0.14	0.06	1.17	0.08	0.06	0.20	**0.01**	1.72
CJ-206-300	300	9.63	0.06	0.02	1.32	0.12	0.06	0.08	**0.01**	1.67
CJ-207-300	300	9.76	0.15	0.06	1.29	0.08	0.06	0.21	**0.01**	1.86
CJ-208-300	300	9.64	-0.02	0.05	1.16	0.13	0.05	0.03	**0.01**	1.41
CJ-209-300	300	9.88	0.21	0.04	1.30	0.09	0.06	0.24	**0.01**	1.95
CJ-210-300	300	9.83	0.47	0.05	0.72	0.10	0.06	0.53	**0.01**	1.94
Means			0.05	0.23	1.01	0.08	0.11	0.21	0.03	1.71

Water Soluble Minerals: For entry to PHREEQE; From NETPATH results							
Based on 7500 g rock/L (multiplier is 0.375)							
Calcite	**Gypsum**	**Nahcolite**	**Halite**	**Sylvite**	**Exchange**	**Dolomite**	**Total**
CaCO3	**CaSO4**	**NaHCO3**	**NaCl**	**KCl**	**Ca/Na**	**CaMg(CO3)2**	
mol/Lgw	**mol/Lgw**	**mol/Lgw**	**mol/Lgw**	**mol/Lgw**	**mol/Lgw**	**mol/Lgw**	**mol/Lgw**
-0.0788	0.3075	0.0413	-0.0075	0.0938	0.1538	0.0525	0.5625
0.0075	0.0638	0.2063	-0.0413	0.1463	0.0788	0.0113	0.4725
-1.0125	1.6125	0.9750	0.0150	0.0188	-0.4200	0.1238	1.3125
-0.3450	0.6675	0.2438	0.0075	0.0188	0.0863	0.1088	0.7875
0.0450	0.0600	0.1913	-0.0150	0.0638	0.1125	0.0075	0.4650
-0.0825	0.0863	0.3113	0.0338	0.0225	0.0038	0.0113	0.3863
0.1050	0.1163	0.3713	-0.0038	0.0450	0.2250	0.0038	0.8625
-0.0300	0.0638	0.2288	0.0525	0.0150	0.0300	0.0075	0.3675
-0.1725	0.3188	0.2100	-0.0113	0.0375	0.1538	0.0563	0.5925
0.0563	0.0600	0.3638	0.0225	0.0300	0.1163	0.0038	0.6525
0.0525	0.0300	0.1950	0.0450	0.0263	0.0750	0.0038	0.4275
0.0675	0.0150	0.4013	0.0188	0.1650	0.0825	0.0038	0.7538
0.0900	0.0300	0.2100	0.0300	0.1575	0.1163	0.0038	0.6375
0.1350	0.0188	0.3413	0.0038	0.0525	0.1538	0.0038	0.7088
0.0450	0.0263	0.4913	0.0338	0.0450	0.0713	0.0038	0.7163
-0.0150	0.0338	0.2813	0.0450	0.0225	0.0225	0.0113	0.4013
-0.0375	0.0150	0.4463	0.0375	0.0225	-0.0188	0.0038	0.4688
0.0075	0.0450	0.2400	0.0488	0.0188	0.0488	0.0038	0.4125
0.0863	0.0300	0.4388	0.0263	0.0263	0.1163	0.0038	0.7275
-0.0413	0.0375	0.2888	0.0563	0.0188	-0.0113	0.0038	0.3525
0.0900	0.0188	0.3450	0.0338	0.0413	0.1088	0.0038	0.6413
0.1125	0.0225	0.3900	0.0150	0.0338	0.1313	0.0038	0.7088
0.0713	0.0225	0.3638	0.0413	0.0300	0.0900	0.0038	0.6225
0.0600	0.0225	0.4013	0.0413	0.0450	0.0825	0.0038	0.6563
0.0525	0.0225	0.5138	0.0188	0.0450	0.0788	0.0038	0.7350
0.0375	0.0188	0.4875	0.0375	0.0300	0.0563	0.0038	0.6713
0.0075	0.0225	0.4463	0.0338	0.0300	0.0300	0.0038	0.5738
0.0675	0.0225	0.4988	0.0338	0.0300	0.0938	0.0038	0.7500
0.1050	0.0263	0.2550	0.0488	0.0225	0.1313	0.0038	0.5925
0.0525	0.0225	0.3938	0.0450	0.0225	0.0750	0.0038	0.6150
0.1163	0.0113	0.3413	0.0300	0.0413	0.1313	0.0038	0.6750
0.0638	0.0188	0.3900	0.0338	0.0300	0.0825	0.0038	0.6225
0.1013	0.0225	0.3975	0.0225	0.0450	0.1238	0.0038	0.7163
0.0600	0.0225	0.3075	0.0488	0.0300	0.0825	0.0038	0.5550
0.0863	0.0338	0.4463	0.0300	0.0263	0.1200	0.0038	0.7463
0.0338	0.0188	0.4538	0.0450	0.0263	0.0525	0.0038	0.6338
0.0525	0.0225	0.4650	0.0338	0.0225	0.0750	0.0038	0.6750
0.0788	0.0150	0.4650	0.0300	0.0263	0.0938	0.0038	0.7125
0.0338	0.0225	0.4650	0.0413	0.0225	0.0563	0.0038	0.6450
0.0563	0.0188	0.4500	0.0413	0.0225	0.0713	0.0038	0.6638
0.1388	0.0150	0.3675	0.0225	0.0638	0.1538	0.0038	0.7650
0.0938	0.0150	0.3863	0.0150	0.1050	0.1088	0.0038	0.7275
0.0713	0.0150	0.3675	0.0413	0.0300	0.0863	0.0038	0.6150
0.0900	0.0188	0.4088	0.0263	0.0300	0.1088	0.0038	0.6863
0.0525	0.0225	0.4388	0.0300	0.0225	0.0750	0.0038	0.6450
0.0225	0.0075	0.4950	0.0450	0.0225	0.0300	0.0038	0.6263
0.0563	0.0225	0.4838	0.0300	0.0225	0.0788	0.0038	0.6975
-0.0075	0.0188	0.4350	0.0488	0.0188	0.0113	0.0038	0.5288
0.0788	0.0150	0.4875	0.0338	0.0225	0.0900	0.0038	0.7313
0.1763	0.0188	0.2700	0.0375	0.0225	0.1988	0.0038	0.7275
Means							
0.0199	0.0847	0.3779	0.0287	0.0406	0.0781	0.0109	0.6406

Single Point Kd's													
Volume of SPF1 = 100 mL													
Mean Labile U (from Sequential Batch Tests) = 0.0436 ug/g													
Sample	Mass	U	U	U	Cs	Cs	Cs	Rd	Rd	Rd		Log U	Log Rd
	(g)	(ug/L)	(ug/L)	(ug/L)	(ug/g)	(ug/g)	(ug/g)	mL/g	mL/g	mL/g		(mol/L)	(mL/g)
		Meas.	Max	Min	Meas.	Min	Max	Meas.	Min	Max		Meas.	Meas.
			2.5% Error	2.5% Error		2.5% Error	2.5% Error		2.5% Error	2.5% Error			
CJ 201-40	5	898	920.45	875.55	-1.3284	-2.1920	-0.4646	-1.48	-2.38	-0.53		-5.423301	#NUM!
CJ 203-40	5	892.2	914.51	869.90	-1.2124	-2.0731	-0.3515	-1.36	-2.27	-0.40		-5.426115	#NUM!
CJ 204-40	5	890.9	913.17	868.63	-1.1864	-2.0465	-0.3261	-1.33	-2.24	-0.38		-5.426748	#NUM!
CJ 206-40	5	906.1	928.75	883.45	-1.4904	-2.3581	-0.6226	-1.64	-2.54	-0.70		-5.419401	#NUM!
CJ 209-40	5	926.6	949.77	903.44	-1.9004	-2.7783	-1.0223	-2.05	-2.93	-1.13		-5.409685	#NUM!
CJ 201-105	5	850.1	871.35	828.85	-0.3704	-1.2101	0.4695	-0.44	-1.39	0.57		-5.447107	#NUM!
CJ 202-105	5	839.4	860.39	818.42	-0.1564	-0.9907	0.6781	-0.19	-1.15	0.83		-5.452608	#NUM!
CJ 203-105	5	821.2	841.73	800.67	0.2076	-0.6176	1.0330	0.25	-0.73	1.29		-5.462128	-0.682773
CJ 204-105	5	822.4	842.96	801.84	0.1836	-0.6422	1.0096	0.22	-0.76	1.26		-5.461494	-0.736127
CJ 205-105	5	839.3	860.28	818.32	-0.1544	-0.9886	0.6801	-0.18	-1.15	0.83		-5.45266	#NUM!
CJ 206-105	5	852.1	873.40	830.80	-0.4104	-1.2511	0.4304	-0.48	-1.43	0.52		-5.446086	#NUM!
CJ 207-105	5	798	817.95	778.05	0.6716	-0.1420	1.4854	0.84	-0.17	1.91		-5.474574	-0.172889
CJ 208-105	5	805.6	825.74	785.46	0.5196	-0.2978	1.3372	0.64	-0.36	1.70		-5.470457	-0.284331
CJ 209-105	5	813.6	833.94	793.26	0.3596	-0.4618	1.1812	0.44	-0.55	1.49		-5.466166	-0.44418
CJ 210-105	5	819.4	839.89	798.92	0.2436	-0.5807	1.0681	0.30	-0.69	1.34		-5.463081	-0.613323
SPF1	0	829.4	850.14	808.67									

Single Point Kd's SPF 2													
Mean Labile U (from Sequential Batch Tests) = 0.0436 ug/g													
Sample	Mass	U	U	U	Cs	Cs	Cs	Rd	Rd	Rd		Log U	Log Rd
	(g)	(ug/L)	(ug/L)	(ug/L)	(ug/g)	(ug/g)	(ug/g)	mL/g	mL/g	mL/g		(mol/L)	(mL/g)
		Meas.	Max	Min	Meas.	Min	Max	Meas.	Min	Max		Meas	Meas.
			2.5% Error	2.5% Error		2.5% Error	2.5% Error		2.5% Error	2.5% Error			
CJ-202-40	5	760.4	779.41	741.39	0.2196	-0.5452	0.9844	0.29	-0.70	1.33		-5.49553	-0.65837
CJ-205-40	5	765	784.13	745.88	0.1276	-0.6395	0.8947	0.17	-0.82	1.20		-5.49292	-0.89415
CJ-207-40	5	756.1	775.00	737.20	0.3056	-0.4571	1.0683	0.40	-0.59	1.45		-5.498	-0.51485
CJ-208-40	5	789.5	809.24	769.76	-0.3624	-1.1418	0.4169	-0.46	-1.41	0.54		-5.47922	#NUM!
CJ-208-40Dup	5	752.1	770.90	733.30	0.3856	-0.3751	1.1463	0.51	-0.49	1.56		-5.5003	-0.41386
CJ-210-40	5	761	780.03	741.98	0.2076	-0.5575	0.9727	0.27	-0.71	1.31		-5.49519	-0.68277
SPF2	0	769.2	788.43	749.97									

Single Point Kd's SPF 3													
Mean Labile U (from Sequential Batch Tests) = 0.0436 ug/g													
Sample	Mass	U	U	U	Cs	Cs	Cs	Rd	Rd	Rd		Log U	Log Rd
	(g)	(ug/L)	(ug/L)	(ug/L)	(ug/g)	(ug/g)	(ug/g)	mL/g	mL/g	mL/g		(mol/L)	mL/g
		Meas	Max	Min	Meas.	Min	Max	Meas.	Min	Max		Meas.	Meas.
			2.5% Error	2.5% Error		2.5% Error	2.5% Error		2.5% Error	2.5% Error			
CJ-202-40	5	742.2	760.76	723.65	1.4236	0.6469	2.2003	1.92	0.85	3.04		-5.50606	0.282867
CJ-205-40	5	756.7	775.62	737.78	1.1336	0.3496	1.9176	1.50	0.45	2.60		-5.49765	0.175536
CJ-207-40	5	783.4	802.99	763.82	0.5996	-0.1977	1.3969	0.77	-0.25	1.83		-5.48259	-0.11612
CJ-208-40	5	797	816.93	777.08	0.3276	-0.4765	1.1317	0.41	-0.58	1.46		-5.47512	-0.38611
CJ-210-40	5	793.9	813.75	774.05	0.3896	-0.4130	1.1922	0.49	-0.51	1.54		-5.47681	-0.30915
SPF 3	0	811.2	831.48	790.92									

Six point Isotherms													
SPF 1 w/U; prepared 2/10/06, Spiked with U on 2/11/06, pH adjusted													
Volume SPF 1 = 100 mL													
Mean Labile U (from Sequential Batch Tests) = 0.0436 ug/g						0.0436							
Sample	Mass	U	U	U	Cs	Cs	Cs	Rd	Rd	Rd		U	Rd
	(g)	(ug/L)	(ug/L)	(ug/L)	(ug/g)	(ug/g)	(ug/g)	mL/g	mL/g	mL/g		Log mol/L	Log mL/g
		Meas.	Max	Min	Meas.	Min	Max	Meas.	Min	Max		meas	meas
			2.5% Error	2.5% Error		2.5% Error	2.5% Error		2.5% Error	2.5% Error			
SPF 1	0	942.30	965.86	918.74									
	0	942.30	965.86	918.74									
CJ 202-40	1	810.80	831.07	790.53	0.67	-3.40	4.74	0.83	-4.09	6.00		-5.467663	-0.080512
	2	799.30	819.28	779.32	0.93	-1.09	2.95	1.17	-1.33	3.79		-5.473867	0.067451
	5	805.40	825.54	785.27	0.28	-0.53	1.09	0.34	-0.65	1.39		-5.470565	-0.462592
	10	764.30	783.41	745.19	0.57	0.18	0.97	0.75	0.22	1.30		-5.493313	-0.126172
	20	708.80	726.52	691.08	0.59	0.39	0.78	0.83	0.54	1.12		-5.526053	-0.083294
	25	696.20	713.61	678.80	0.53	0.38	0.68	0.76	0.53	1.00		-5.533843	-0.120759
CJ 205-40	1	821.40	841.94	800.87	-0.39	-4.48	3.71	-0.47	-5.32	4.63		-5.462022	
	2	799.10	819.08	779.12	0.94	-1.08	2.96	1.18	-1.31	3.80		-5.473976	0.072187
	5	793.90	813.75	774.05	0.51	-0.30	1.31	0.64	-0.37	1.70		-5.476811	-0.194244
	10	766.00	785.15	746.85	0.55	0.16	0.95	0.72	0.20	1.27		-5.492348	-0.140249
	20	718.80	736.77	700.83	0.54	0.34	0.73	0.74	0.47	1.04		-5.519969	-0.128173
	25	714.40	732.26	696.54	0.45	0.30	0.61	0.64	0.41	0.87		-5.522636	-0.196503
CJ 207-40	1	808.40	828.61	788.19	0.91	-3.15	4.98	1.13	-3.80	6.32		-5.468951	0.05313
	2	811.90	832.20	791.60	0.30	-1.73	2.34	0.37	-2.08	2.96		-5.467074	-0.427201
	5	811.60	831.89	791.31	0.15	-0.66	0.97	0.19	-0.79	1.22		-5.467235	-0.722951
SPF1	0	817.10	837.53	796.67								-5.464302	
	10	718.20	736.16	700.25	0.65	0.27	1.02	0.90	0.37	1.46		-5.520332	-0.044939
	20	704.60	722.22	686.99	0.41	0.23	0.60	0.59	0.32	0.87		-5.528634	-0.231362
	25	704.40	722.01	686.79	0.34	0.19	0.49	0.48	0.27	0.71		-5.528758	-0.31583
CJ 208-40	1	775.40	794.79	756.02	0.36	-3.52	4.25	0.47	-4.43	5.62		-5.487051	-0.328902
	2	747.30	765.98	728.62	1.61	-0.30	3.52	2.15	-0.39	4.83		-5.503082	0.332953
	5	753.60	772.44	734.76	0.54	-0.22	1.31	0.72	-0.29	1.78		-5.499436	-0.141861
	10	753.70	772.54	734.86	0.29	-0.09	0.68	0.39	-0.12	0.92		-5.499378	-0.410924
	20	729.40	747.64	711.17	0.29	0.10	0.48	0.40	0.14	0.67		-5.513611	-0.401167
	25	734.20	752.56	715.85	0.22	0.07	0.37	0.30	0.09	0.52		-5.510763	-0.521029
CJ 210-40	1	766.80	785.97	747.63	1.22	-2.64	5.09	1.60	-3.36	6.80		-5.491895	0.202957
	2	751.70	770.49	732.91	1.39	-0.52	3.30	1.85	-0.68	4.50		-5.500532	0.266533
	5	757.60	776.54	738.66	0.46	-0.30	1.23	0.61	-0.39	1.67		-5.497137	-0.213297
	10	732.40	750.71	714.09	0.51	0.13	0.88	0.69	0.17	1.24		-5.511829	-0.160941
	20	705.80	723.45	688.16	0.41	0.22	0.59	0.58	0.31	0.86		-5.527895	-0.238447
	25	735.40	753.79	717.02	0.22	0.07	0.37	0.29	0.09	0.51		-5.510053	-0.531266
SPF1	0	778.60	798.07	759.14									

Sequential Batch leaching																
Leach solution is SPF1																
Placed on orbital shaker table X 24 hours																
Centrifuge 20" X 3500RPM																
Filtered through 0.45um filter																
50 mL split retained, balance placed with same proportion of next soil to be tested (4:1)																
Sample	Vol	Mass	pH	ORP	Conducti	Alkalin	Chloride	Nitrate	Sulfate	NH3-N	U	Ca	Na	Mg	K	
	SPF1	(g)		mV	(uS/cm)	(mg/L a	(mg/L)	(mg/L)	(mg/L)	(mg/L)	(ug/L)	(mg/L)	(mg/L)	(mg/L)	(mg/L)	
	(mL)					CaCO3)										
CJ 203-40	400	100	7.66	196.7	29400	560	1026	764	18676	1700	5.5	320	5700	440	141	
CJ 204-40	315	78.75	7.79	186.3	30100	450	1096	828	19872	1500	19.3	350	5400	510	156	
CJ 206-40	240	60	7.83	175.2	29900	560	1120	820	19910	1300	25.4	349	6300	300	177	
CJ 205-40	400	100	7.73	187.3	29200	620	1106	756	18504	1600	3	236	5700	210	141	
CJ 205-105	315	78.75	7.85	171.4	29800	560	1116	770	18828	1400	19.5	220	6400	200	168	
CJ 205-170	240	60	7.96	171.5	29600	520	1196	776	19032	1100	29	199	6500	250	157	
CJ 205-235	165	41.25	7.85	173.3	29700	400	1284	804	19700	1800	44.9	203	7000	180	167	
CJ 205-300	100	25	7.97	173.5	30600	330	1336	794	19492	900	54.5	196	7800	180	166	
SPF1 (start)			6.62	197.4	26800	560				2000	<0.1					
SPF1 (Final)			7.85	191.9	29600	510	1018	738	18272			196	5300	310	129	

Appendix D

Dr. William C. Hood, 2006

X-Ray Diffraction Analysis Determination of the Mineralogy of 10 Mancos Shale Samples

Prepared for S.M. Stoller Corporation, February 3, 2006
Grand Junction, Colorado

X-ray determination of the mineralogy of 10 Mancos Shale samples

A report prepared by:

William C. Hood, PhD
AAPG Certified Professional Geologist No. 2185
February 3, 2006

X-ray determination of the mineralogy of 10 Mancos Shale samples

Introduction

At the request of Stan Morrison, ten samples of Mancos Shale from the proposed Atlas Mill tailings disposal site near Crescent Junction were examined by x-ray diffraction techniques. The purpose of the examination was to identify the minerals present in the shale, with special emphasis on the clay mineralogy.

Summary and Conclusions

The mineralogy of the ten samples is quite similar, as might be expected in a marine environment such as the Mancos Shale. The non-phyllosilicate minerals identified include quartz, calcite, dolomite, orthoclase, plagioclase and gypsum. These minerals are estimated to comprise from a third to one-half of the total sample. The clay minerals identified, in order of abundance, are mixed-layer illite/smectite (a little less than 38 percent, discrete illite (about 33 percent), kaolinite (about 28 percent) and mixed-layer chlorite/vermiculite (perhaps 2 or 3 percent). The mixed-layer illite/smectite contains at least 60 percent illitic layers, but the actual amount could not be determined with accuracy. Kaolinite crystallites are the largest clay minerals in the samples at an average grain size of 297 A, followed by illite at 152 A and mixed-layer illite/smectite at 67 A.

Methods

The samples were supplied in pulverized form. A portion of each of the 10 original samples was ground for several minutes using a porcelain mortar and pestle. A five-gram sample of this material was removed for clay analysis. The technique used to separate clay minerals is described in Appendix 1. About two grams of the remaining material was ground for several more minutes to obtain a powdered sample for determining the bulk mineralogy.

The powdered bulk samples were loaded into sample holders and scanned from 4.2 to 50 degrees two-theta using the Rigaku Miniflex x-ray diffractometer at Mesa State College.

Clay samples were scanned over the same interval so that direct comparisons of the clay patterns to the bulk samples could be made. Four scans were made of each clay sample: untreated, glycol solvated, heat treated to 300° C and heat treated to 550° C. Glycol solvation is accomplished by putting the samples into a desiccator that contains ethylene glycol and heating the desiccator in an oven at 60° C overnight. The purpose of this treatment is to expand the mineral smectite or smectite layers within mixed-layer clays to approximately 17 Angstroms d-spacing, facilitating the identification of clays containing an expandable smectitic component. The two heat treatments were accomplished by placing the samples into a muffle furnace and heating to the appropriate temperature, as indicated by a thermocouple thermometer. The 300° C heat treatment collapses the expandable layers to 9.2 Angstroms but does not destroy chlorite, chlorite layers in mixed-layer clays or kaolinite. The 550° C heat treatment destroys kaolinite, facilitating its distinction from chlorite.

Results

Bulk samples. The minerals identified in the bulk samples are, in order of general abundance, quartz, dolomite, calcite, plagioclase, orthoclase and gypsum. The estimated abundances of these minerals are given in Table 1 and the method of estimating the abundances is explained in Appendix 2, which also includes diffraction patterns for quartz, calcite, dolomite, albite and gypsum standards.

Table 1. Estimated abundances (in percent) of non-phyllosilicate minerals in bulk Mancos Shale samples.

Sample	Quartz	Calcite	Dolomite	Orthoclase	Plagioclase	Gypsum
CJ201-40	32	3	5	1	1	Tr
CJ202-40	29	3	4	1	1	1
CJ203-40	36	4	5	1	2	1
CJ204-40	33	2	3	1	1	
CJ205-40	28	3	6	1	1	
CJ206-40	39	4	6	1	2	
CJ207-40	25	3	3	1	1	
CJ208-40	38	3	5	1	1	
CJ209-40	27	1	3	2	1	Tr
CJ210-40	24	4	3	1	1	

Minerals were identified using the diffraction peaks listed in Appendix 3. The x-ray patterns for the bulk samples themselves are in Appendix 4. For each sample, two copies of the x-ray diffraction patterns are included, one with d-spacings for most of the peaks and one with most of the peaks identified as to which mineral they result from.

To verify the presence of the carbonate minerals, calcite and dolomite, a small amount of sample CJ-205-40 was placed in a small container, mixed with water and then several drops of dilute hydrochloric acid were added. The sample effervesced vigorously, confirming the presence of carbonate minerals. After the effervescence stopped, the sample was washed twice to remove the dissolved constituents, dried and x-rayed. The peaks associated with calcite disappeared and the dolomite peak was considerably reduced in intensity, confirming the presence of both minerals (Figure 1).

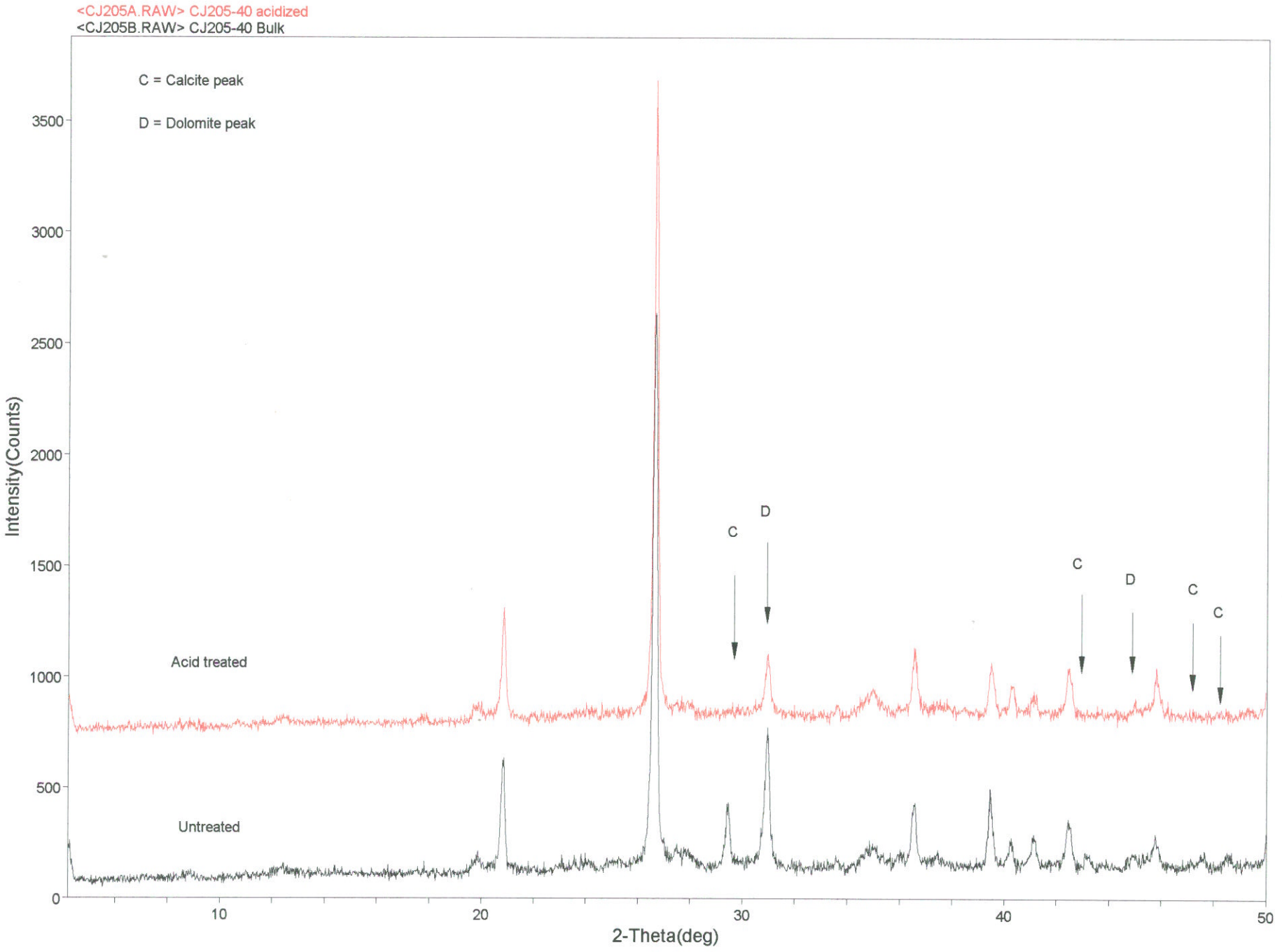

Fig. 1. Comparison of sample CJ201-40 before and after acid treatment.

Clay separates.

Identification of clay minerals.

Examination of a typical x-ray diffraction pattern reveals the presence of four phyllosilicate and two non-phyllosilicate minerals in these samples. The two non-phyllosilicates are quartz and dolomite. The phyllosilicate minerals identified are kaolinite, illite, mixed-layer illite/smectite and mixed-layer chlorite/vermiculite. The following paragraphs explain how these minerals were identified.

Kaolinite is recognized by peaks at approximately 7.14 Angstroms, 3.57 Angstroms and 2.38 Angstroms. These correspond to the first, second and third order diffractions from the (001) plane. These spacings do not change when the sample is glycol-solvated or heated to 300° C. They disappear upon heating the sample to 550° C, indicating that the kaolinite has been destroyed. Kaolinite is present in all of the samples.

Illite is recognized by peaks at approximately 10 Angstroms, 5.0 Angstroms, 3.3 Angstroms, 2.5 Angstroms and 2.0 Angstroms. These represent the first, second, third, fourth and fifth order diffractions from the (001) plane. Peak intensities are strongest for the odd orders, with the third order peak being the strongest, as is typical for a dioctahedral phyllosilicate. In the case of the CJ sample set, the peak at 3.3 Angstroms (3rd order) is quite strong because it is combined with the most intense peak for quartz. The fourth order peak at 2.5 Angstroms is very weak, hardly rising above background in most of the samples. Glycol solvation shifts the peak of expandable minerals, making the 10 Angstrom peak quite obvious. Heat treatments bring about slight peak shifts and significant increases in intensity. These changes are not so much due to changes in the illite itself, but are mainly a result of the collapse of mixed-layer clays to 9.9 Angstroms or slightly less and the diffraction from that material being added to that of the discrete illite.

Mixed-layer illite/smectite is recognized by a broad peak between about 11.2 and 11.9 Angstroms in the untreated sample. The peak is broad and there is enough "chatter" in the background that it is difficult to pick the center of the peak with any certainty. Another complication is that the peak overlaps the peaks from illite and chlorite. The additive effects of these peaks can cause the apparent peak position to shift. In the glycol-solvated sample, the peak shifts to higher d-spacing (lower angle 2-theta or left on the diffraction pattern), indicating expansion of smectitic layers. In these samples, the shift does not usually result in a well-developed peak, but rather a significant drop in intensity near the 10 Angstrom illite peak and a smeared-out low hump between 14 and 17 Angstroms. Heating to 300° C collapses the expandable layers to approximately 9.9 Angstroms, resulting in a marked increase in intensity of the peak at approximately 10 Angstroms. This peak is asymmetric toward low angles, suggesting that not all of the layers are totally collapsed. Heating to 550° collapses these layers and sharpens the peak at approximately 10 Angstroms.

The presence of small amounts of a chlorite component in the CJ samples is recognized by a low, broad peak about 14.3 Angstroms and a sharper, third order peak, at 4.8 Angstroms, which appears as a shoulder or small peak on the high angle side of the second-order illite peak. The 14.3 Angstrom peak is small and sometimes is just a shoulder on the mixed-layer

illite smectite peak. It persists through glycol solvation and low heat and does not seem to change position, although interference from mixed-layer illite/smectite makes the peak position indeterminate. The peak remains after heating to 550° C but shifts to lower d-spacings, typically about 13.5 angstroms. The shift indicates that the material is not a pure chlorite, but rather a mixed-layer material. To summarize its characteristics, it does not seem to expand upon glycol salvation and collapses somewhat with high heat. Based on the material presented in Moore and Reynolds (1997) the mineral is probably a mixed-layer chlorite/vermiculite.

Figure 2 shows the results of the various treatments for sample CJ201-40 combined into one display to show how the patterns change with various treatments. Stacked patterns for all ten of the samples are contained in Appendix 5. The individual x-ray patterns are located in Appendix 6.

Estimating the relative amounts of clay minerals.

To estimate the relative amounts of the various clay minerals, the patterns of the glycol-solvated samples were used. By expanding the smectitic layers in mixed-layer clay, this treatment separates peaks of clays with expandable components from the 10 Angstrom peak of illite. Although the glycol-solvated pattern allows the separation of discrete illite, it does not allow the separation of the mixed-layer illite/smectite from the mixed-layer chlorite/vermiculite.

The first step is to draw a smooth background through the low-angle portion of the x-ray pattern. Figure 3 shows what this looks like. Once the background curve is established, the Jade computer program was used to eliminate the background. Appendix 7 contains the patterns after this step. The next step was to use the peak-painting module within Jade to determine the area under the peak for each of the first-order peaks of mixed-layer clay, discrete illite and kaolinite. Figure 4 shows the painted peaks of a typical sample and Table 2 gives the results of these measurements.

Table 2. Areas under the peaks, as calculated by the Jade computer program.

Sample	Mixed-layer	Illite	Kaolinite	Total
CJ201-40	330	223	214	767
CJ202-40	208	198	141	547
CJ203-40	329	239	194	762
CJ204-40	302	225	220	747
CJ205-40	267	181	134	582
CJ206-40	253	235	200	688
CJ207-40	127	170	177	474
CJ208-40	263	275	216	754
CJ209-40	215	172	160	547
CJ210-40	191	181	123	495

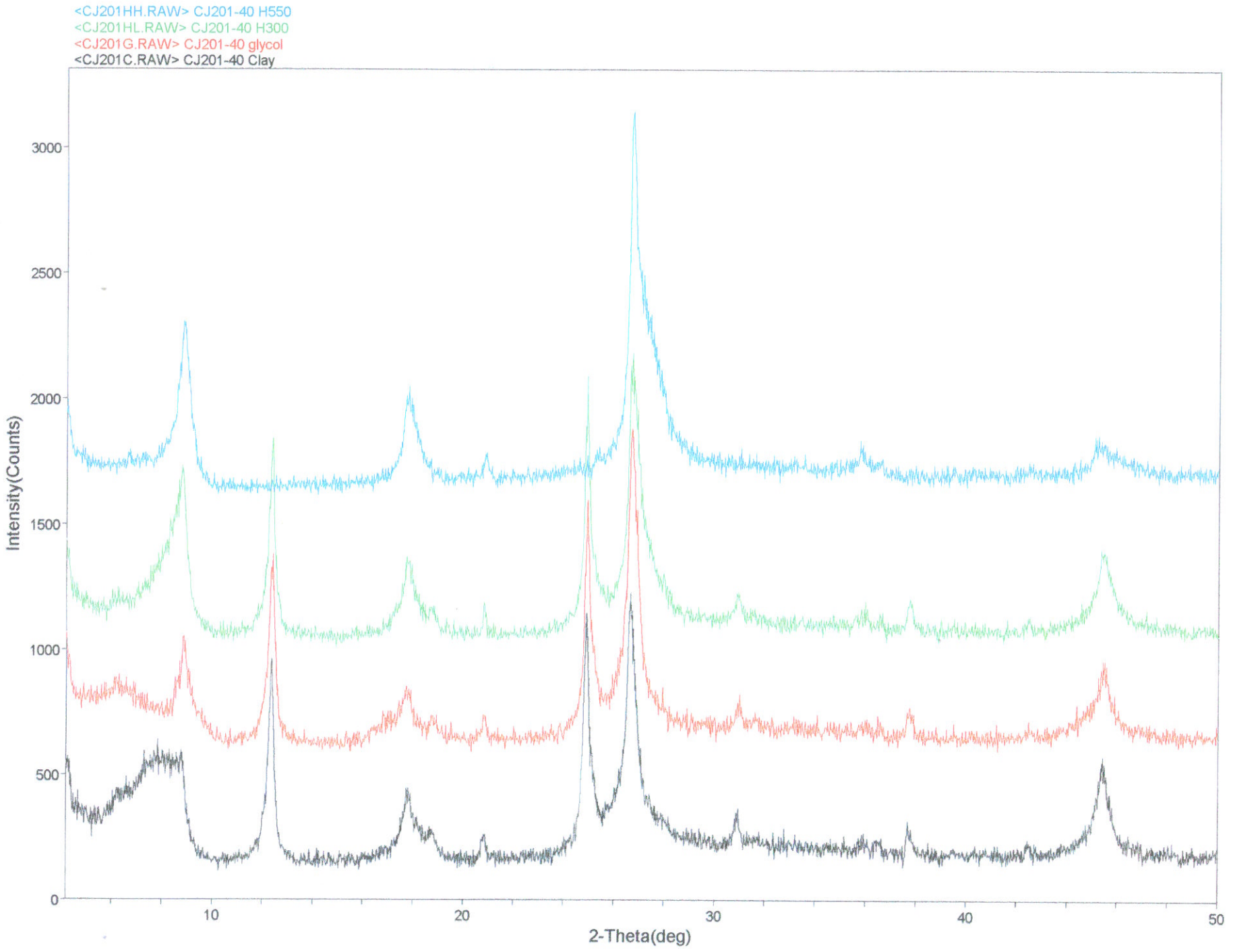

Fig. 2. Stacked x-ray patterns showing effects of various treatments, sample CJ201-40.

Mesa State College

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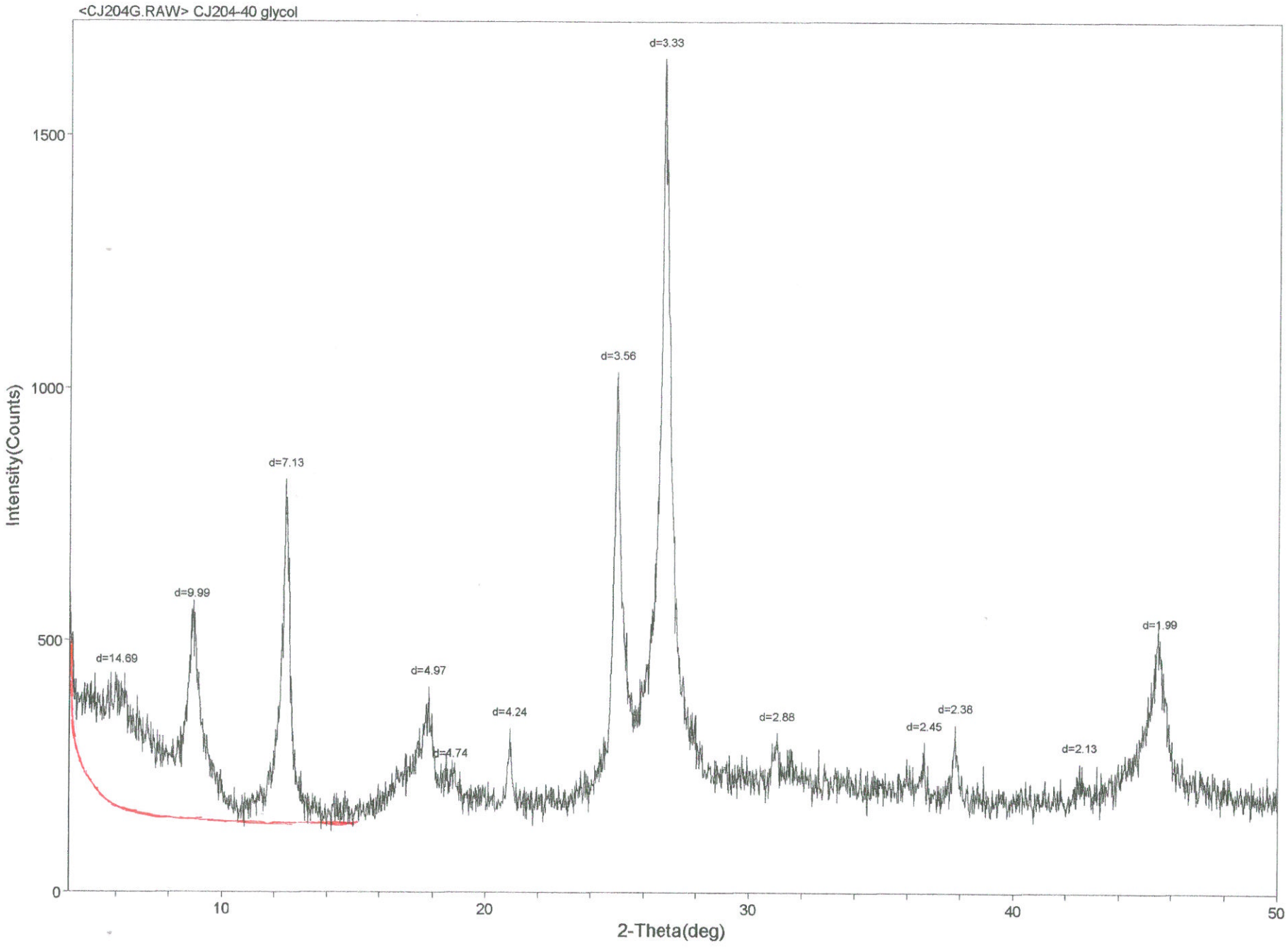

Fig. 3. Estimated low-angle background shown in red, sample CJ204-40.

Mesa State College

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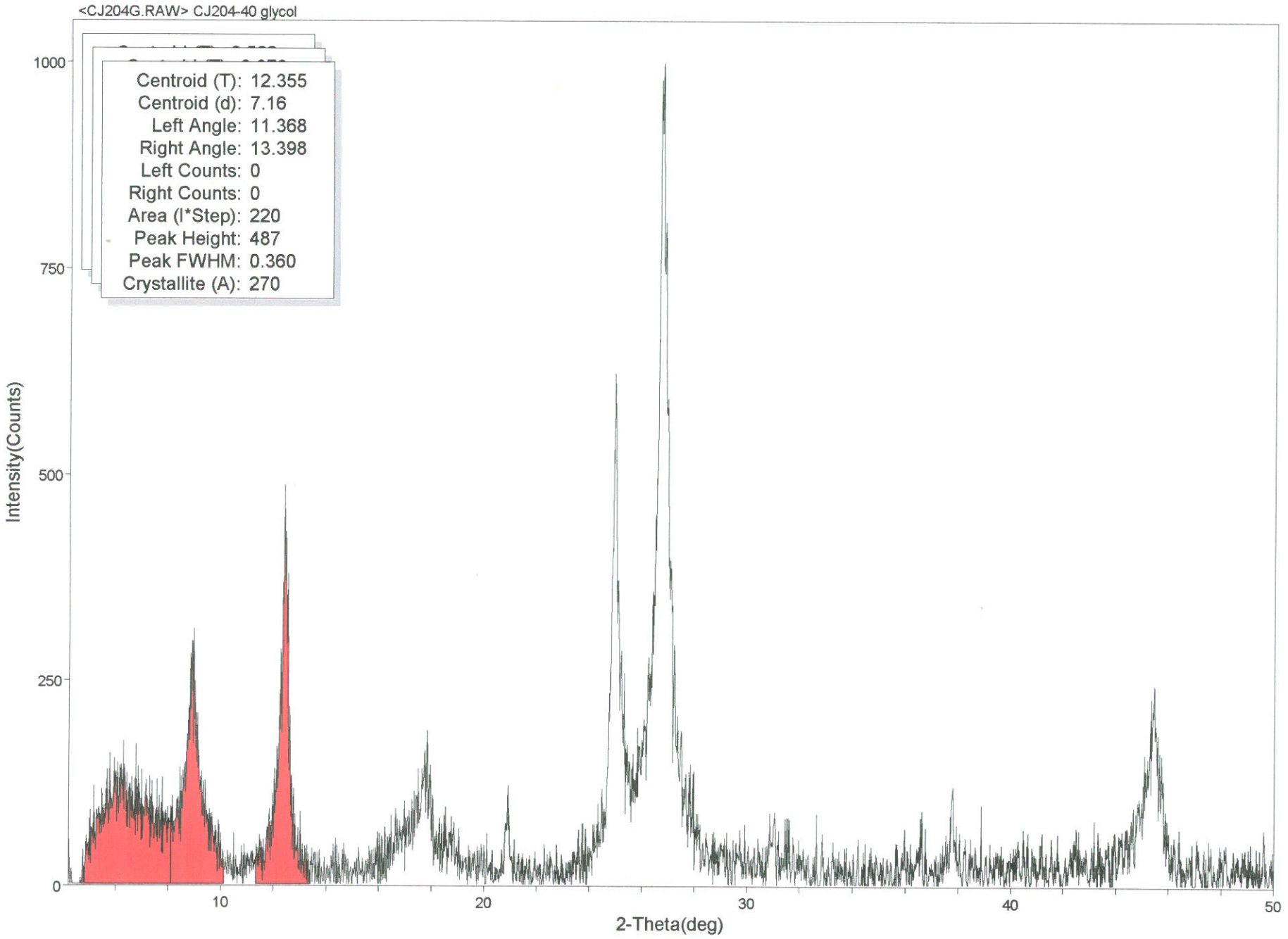

Fig. 4. Measured areas under the peaks, sample CJ204-40.

Finally, the areas under the peaks of the three minerals were added and the relative amounts of the components calculated as a percentage of the total. These values are given in Table 3.

Table 3. Estimated abundance of individual clays, derived from areas under the peaks.

Sample	Mixed-layer	Illite	Kaolinite
CJ201-40	43	29	28
CJ202-40	38	36	26
CJ203-40	43	31	25
CJ204-40	40	30	29
CJ205-40	46	31	23
CJ206-40	37	34	29
CJ207-40	27	36	37
CJ208-40	35	36	29
CJ209-40	39	31	29
CJ210-40	39	37	25

Note: Mixed-layer includes both mixed-layer illite/smectite plus a much smaller amount of mixed-layer chlorite/vermiculite. Mixed-layer chlorite/vermiculite makes up perhaps 5 percent of the mixed-layer component.

The values in Table 3 should be taken only as semi-quantitative approximations. To obtain more quantitative values, standards of similar grain size and crystallinity would have to be mixed in various amounts and x-rayed under the same conditions as the Mancos Shale samples. Such standards were not available. The values that were obtained in this study are, however, useful for inter-sample comparisons.

Little published work exists on the clay mineralogy of the Mancos Shale in the Colorado Plateau region. L. G. Schultz, cited in Eckel, (p. 276) reports that the clays consist of 50 to 60 percent mixed-layer illite/smectite, 12 to 15 percent poorly ordered kaolinite, and 30 to 35 percent discrete illite. No information was given about the method used to determine these amounts. The CJ samples contain more kaolinite and less mixed-layer illite/smectite than reported by Schultz.

Amount of illite in mixed-layer illite/smectite

The amount of illitic and smectitic components in the mixed-layer illite/smectite is very difficult to determine in this sample set due to interference among the peaks of the various minerals. The usual procedure for determining the amount of illite and smectite in a mixed-layered illite/smectite is to use the glycol solvated pattern and determine the peak positions for the (001)/(002) and (002)/(003) peaks. Unfortunately in the CJ sample set, the (001)/(002) peak (between 10.3 and 9.0° 2-theta) lies on the flank of a much stronger illite peak and cannot be resolved. Likewise, the (002)/(003) peak (between 15.8 and 17.4° 2-theta) lies on the flank of the second order illite peak and just appears as a broadening of the illite peak and not as a distinct peak itself. However, this fact by itself suggests that the material is richer in the illite component than the smectite component. Materials with large amounts of smectite have peaks at the low angle end of the range, whereas peaks with a large

amount of illite component have peaks at the high end of the range, close to the peak for pure illite.

In order to get an independent approximation as to the amount of illite layers in the mixed-layer illite/smectite, I examined the position of the (001)/(001) peak in the Mg-saturated but otherwise untreated sample. Pure smectite would have a peak at 14 Angstroms and pure illite a peak at 10 Angstroms. The assumption this method makes is that there is complete randomness in the mixing of illitic and smectitic components and that the peak position varies in a straight-line manner from 14 to 10 Angstroms. Table 4 presents the results of this analysis. The values are rounded to the nearest 10 percent because of the difficulty in picking the peak position.

Table 4. Estimated amounts of illitic layers in mixed-layer illite/smectite.

Sample	**d-spacing**	**% illitic layers**
CJ201-40	11.3	70
CJ202-40	11.6	60
CJ203-40	11.6	60
CJ204-40	11.5	60
CJ205-40	11,7	60
CJ206-40	11.8	60
CJ207-40	11.9	50
CJ208-40	11.8	60
CJ209-40	11.6	60
CJ210-40	11.6	60

The average amount of illitic layers in the material is 60 percent. This should probably be considered to be a minimum estimation, because the (002)/(003) peak of the glycol solvated samples suggest a value that would probably be more on the order of 80 percent illitic layers.

Crystallite size.

The Jade computer program contains an algorithm for determining crystallite size of crystallites smaller than 1 micron. This information is produces as a by-product of measuring the area under a peak and became available by determining the relative amounts of the various clay minerals. In general, kaolinite has the largest grains with an average size of 297 A, followed by illite at 152 A and the mixed-layer material at 67 A (Table 5).

Table 5. Crystallite size of clay minerals in the CJ sample set.

Samples	Mixed-layer	Illite	Kaolinite
CJ201-40	58	159	334
CJ202-40	74	159	337
CJ203-40	54	133	391
CJ204-40	58	149	270
CJ205-40	57	153	281
CJ206-40	65	171	332
CJ207-40	97	171	231
CJ208-40	71	120	274
CJ209-40	76	160	220
CJ210-40	57	148	295

References

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Moore, D. M., and R. C. Reynolds (1997) X-ray diffraction and the identification and analysis of clay minerals, 2nd ed.: Oxford University Press, New York, 378 p.

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Appendix 1.

Method used to separate and prepare clay minerals for x-ray diffraction

Appendix 1. Method used to separate and prepare clay minerals for x-ray diffraction

1. Place bulk sample in water overnight to remove any easily soluble material and to partially disaggregate clay. Remove as much of the water as practical without losing the sample.

2. Add fresh water and ¼ tsp. of sodium metaphosphate (Calgon). Agitate vigorously to get the material into suspension.

3. Allow to sit undisturbed for 8 hrs. With a turkey baster or some other large pipette, remove the upper 10 cm. of the suspension. Place this in a separate container. This suspension contains clay (less than 2 micron particles).

4. Re-suspend the bulk material to collect additional clay. If the original suspension yielded little clay or if it flocculated, add additional Calgon. Otherwise, do not add Calgon.

5. Add ¼ tsp. of magnesium chloride or magnesium sulfate to the clay suspension. This does two things; it flocculates the clay and begins the magnesium saturation process. When the flocculated particles have settled to the bottom of the container, remove as much water as you can with the pipette.

6. After re-suspending the bulk sample, repeat step 3. Add the clay suspension to the container with the flocculated clay. Repeat step 5.

7. Repeat steps 4 and 5, but do not add more Calgon to the bulk sample. If there is insufficient clay to do the required analysis, steps 4 & 5 can be repeated as necessary.

8. When sufficient clay has been collected and step 5 has been completed on the accumulated clay, the clay should by now be Mg saturated. At this point, centrifuge the sample to concentrate the clay and remove as much of the water as possible.

9. Add distilled water and get the flocculated clay into suspension. Centrifuge and remove the water.

10. Repeat step 9 until you are confident that you have removed the excess Mg. This usually takes 3 washings, but it depends on the size of the centrifuge tube. When the excess Mg salt is gone, it will take much longer to clear the sample because the finest fraction of clay will start staying in suspension.

11. Add enough water to make a rather thick suspension of clay and agitate vigorously. Allow to sit for a couple of hours so that clumps of clay will settle out. With a pipette, collect the clay from the top centimeter (to obtain only -2 micron material and not the larger flocs), put it onto a glass slide and allow to dry.

If the sample contains a lot of smectite or if it too thick, it may curl up off of the slide. There are two things that can be done if this happens. Make another slide using less material or frost the glass slide lightly and remake the sample.

Appendix 2.

Estimating the abundance of non-phyllosilicate minerals in Mancos Shale

Appendix 2. Estimating the abundance of non-phyllosilicate minerals in Mancos Shale

The amounts of non-phyllosilicate minerals in the Mancos Shale samples were estimated using the following technique. First, diffraction patterns of pure samples of quartz, calcite, dolomite and albite were obtained under the same conditions as the bulk samples of Mancos Shale. Because the intensities of the most intense peak of the minerals were not identical, the next step was to obtain a normalization factor so that each of the other minerals could be compared to quartz. This was done by first removing the background from the patterns and determining the peak intensity, then dividing the peak intensity of each of the minerals into the peak intensity of quartz. A pure sample of orthoclase was not available, so the intensity of the main peak of this mineral was assumed to be the same as that of albite. This most likely gives an incorrect normalization factor, but because this mineral is present in amounts just slightly above the detection limit, it makes little difference in the interpretation.

The second step is to normalize the peak intensities to quartz and sum the various peak intensities. This gives an approximation of what the quartz peak intensity would be if only quartz plus phyllosilicate minerals were present in the samples. The ratio of intensities of the normalized peaks to the pure quartz standard is a measure of the amount of non-phyllosilicate minerals present in the sample. This assumes that the presence of phyllosilicate minerals suppresses the quartz peak in an amount directly proportional to their abundance. The total amount of non-phyllosilicate minerals is estimated from 33 to 52 percent in the 10 Mancos Shale samples.

The final step is to compare the intensities of the various normalized peaks to the total intensity values and multiply that by the percent of non-phyllosilicate minerals obtained in the preceding step. This gives an approximation of the abundance of each mineral in the bulk sample.

The mineral gypsum was not included in the calculation just described because it was detected in only 4 samples. By comparison with the values for the other minerals, the amount of gypsum is estimated to be 1 percent or less.

The data and results of calculations are shown on the next page. Diffraction patterns for quartz, calcite, dolomite, albite and gypsum follow the calculations page.

Method for calculating abundance of non-phyllosilicate minerals in bulk samples

Normalize calcite, dolomite and feldspar standards to quartz (background removed)

	Pk. Height	Factor
Quartz	6528	1.000
Calcite	7154	0.912
Dolomite	8683	0.752
Albite	7647	0.854

Measured peak heights (in counts/second) after background removed

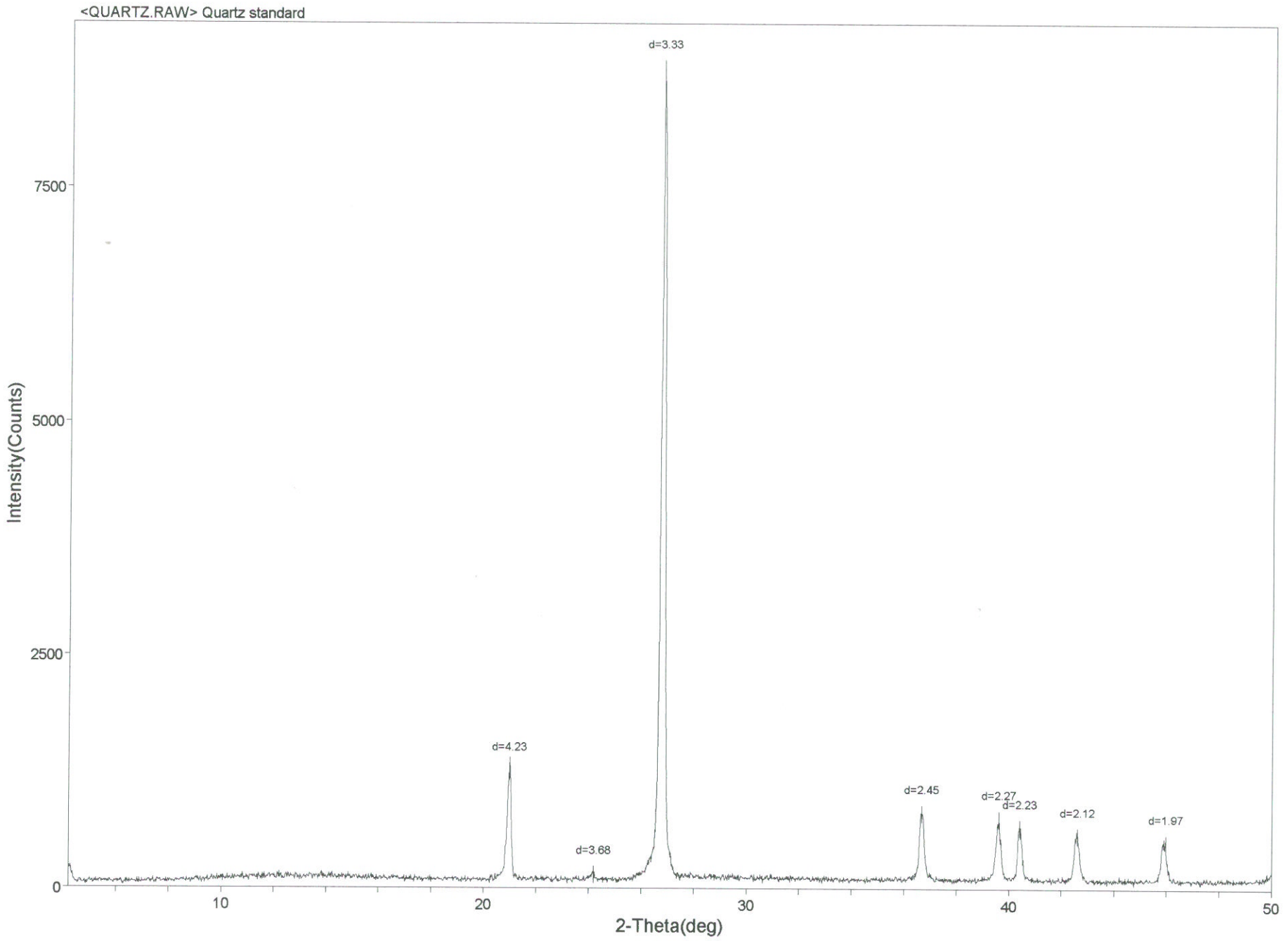
Sample	Quartz	Calcite	Dolomite	Orthoclase	Plagioclase
CJ201-40	2091	199	395	96	68
CJ202-40	1866	240	365	87	86
CJ203-40	2334	283	424	113	121
CJ204-40	2145	178	277	56	102
CJ205-40	1850	233	496	86	90
CJ206-40	2535	251	559	90	128
CJ207-40	1606	213	222	79	104
CJ208-40	2495	241	408	94	94
CJ209-40	1768	88	288	138	114
CJ210-40	1566	268	293	113	93

Peak heights (in counts/second) normalized to quartz

Sample	Quartz	Calcite	Dolomite	Orthoclase	Plagioclase	Total	Percent Non-clay
CJ201-40	2091	182	297	82	58	2710	42
CJ202-40	1866	219	274	74	73	2507	38
CJ203-40	2334	258	319	96	103	3111	48
CJ204-40	2145	162	208	48	87	2651	41
CJ205-40	1850	213	373	73	77	2586	40
CJ206-40	2535	229	420	77	109	3370	52
CJ207-40	1606	194	167	67	89	2123	33
CJ208-40	2495	220	307	80	80	3182	49
CJ209-40	1768	80	217	118	97	2280	35
CJ210-40	1566	245	220	96	79	2207	34

Estimated Percentages of Non-phyllosilicate minerals

Sample	Quartz	Calcite	Dolomite	Orthoclase	Plagioclase	Gypsum
CJ201-40	32	3	5	1	1	Tr
CJ202-40	29	3	4	1	1	1
CJ203-40	36	4	5	1	2	1
CJ204-40	33	2	3	1	1	
CJ205-40	28	3	6	1	1	
CJ206-40	39	4	6	1	2	
CJ207-40	25	3	3	1	1	
CJ208-40	38	3	5	1	1	
CJ209-40	27	1	3	2	1	Tr
CJ210-40	24	4	3	1	1	



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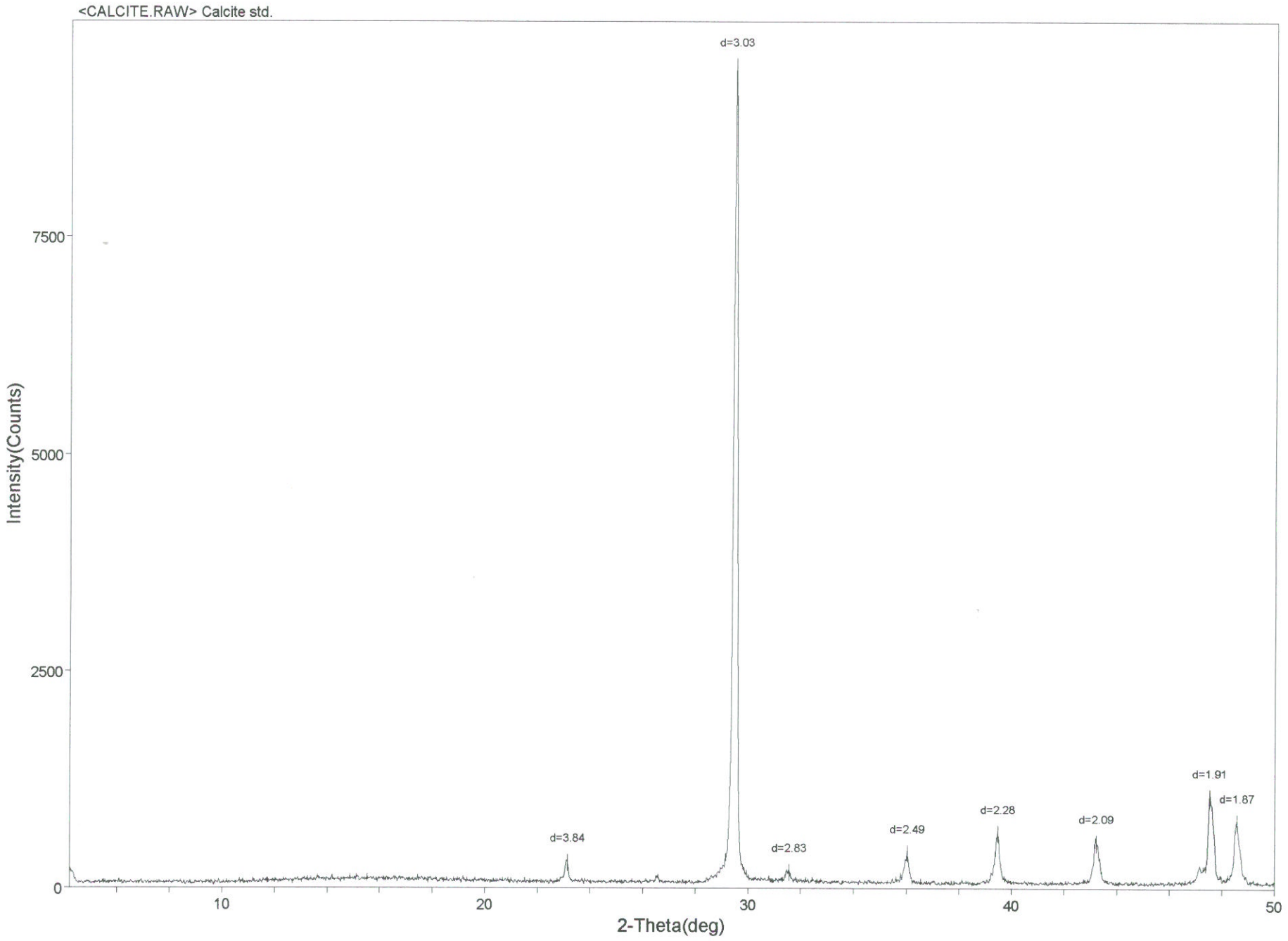

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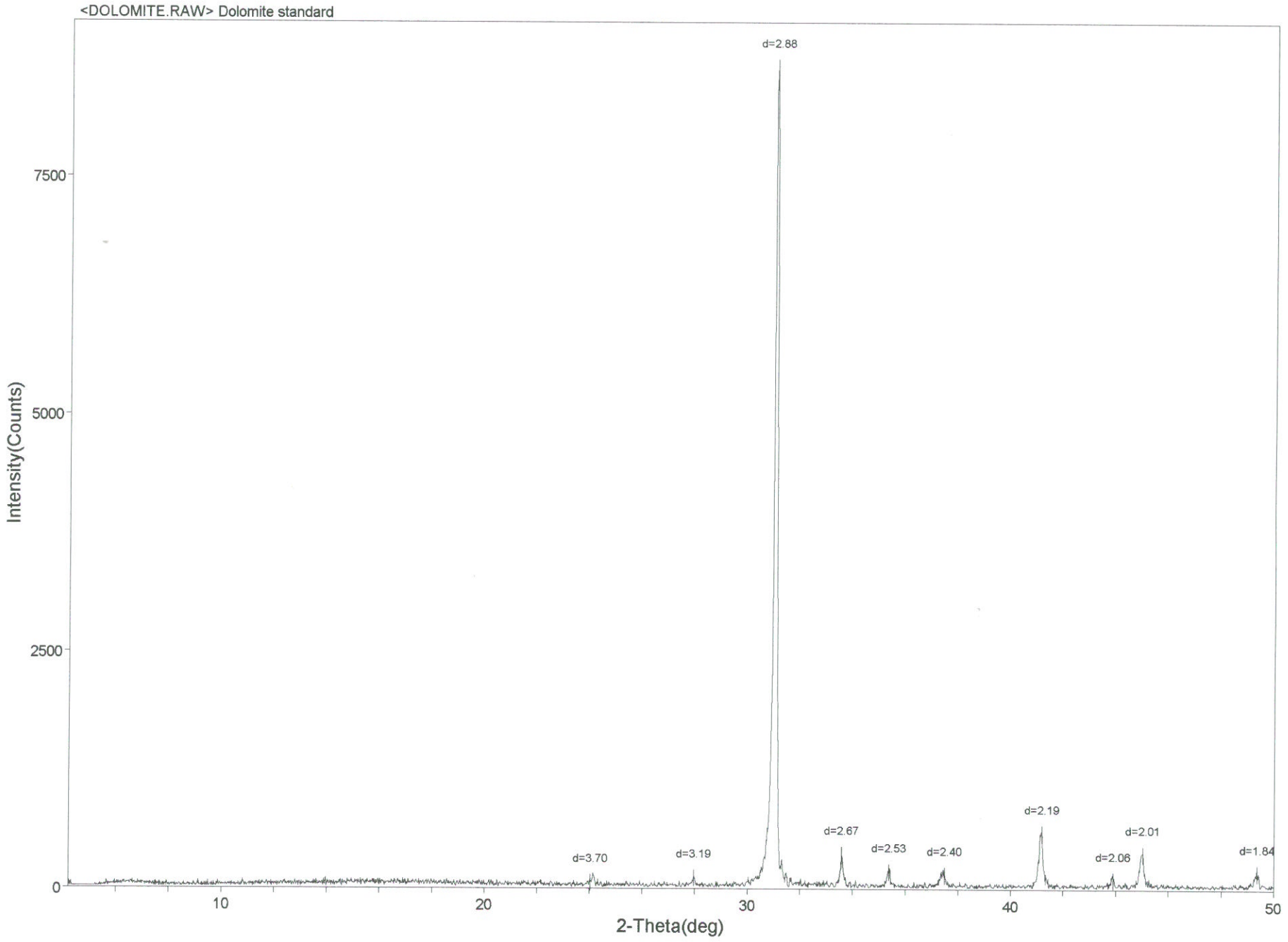

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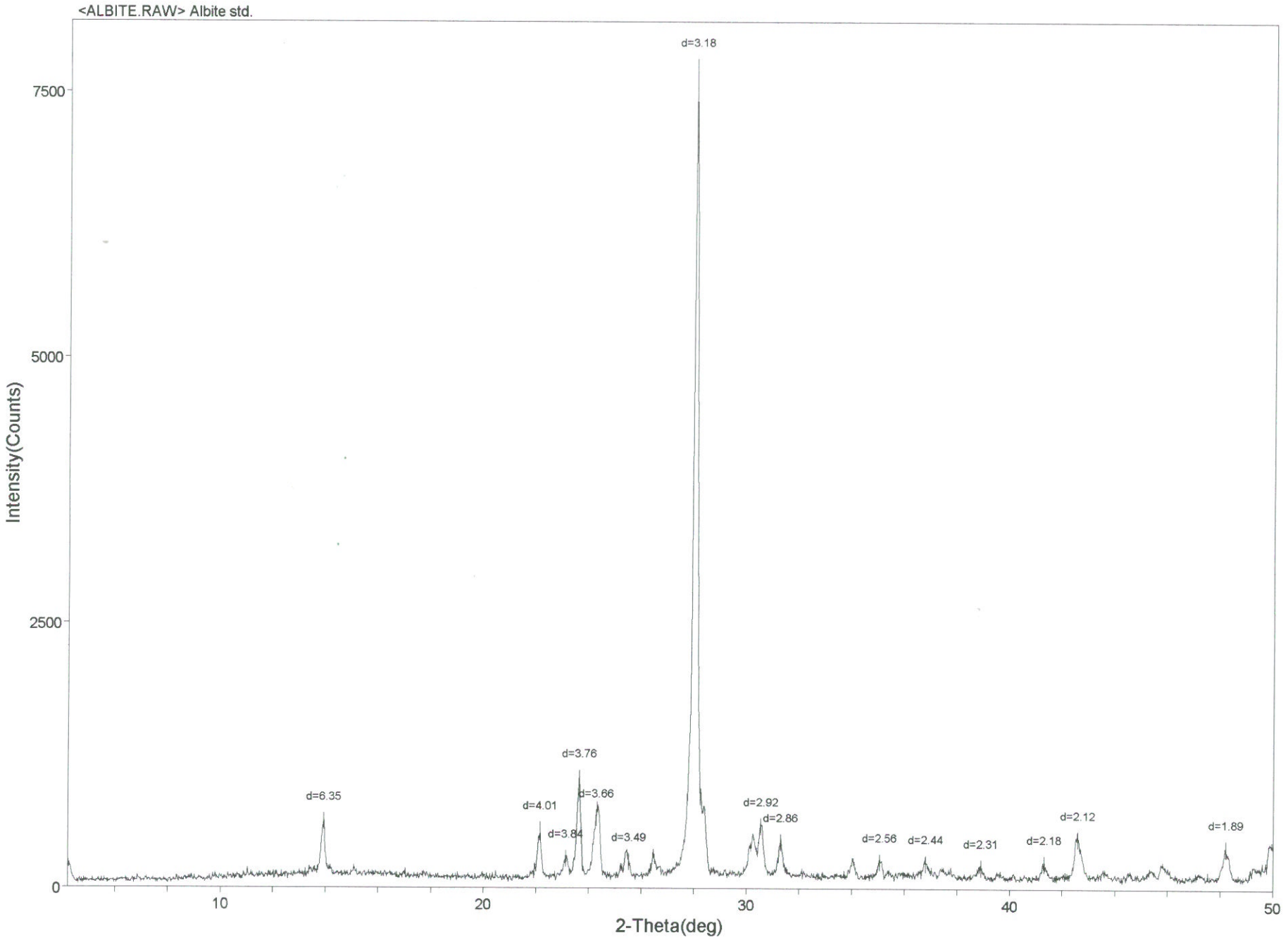

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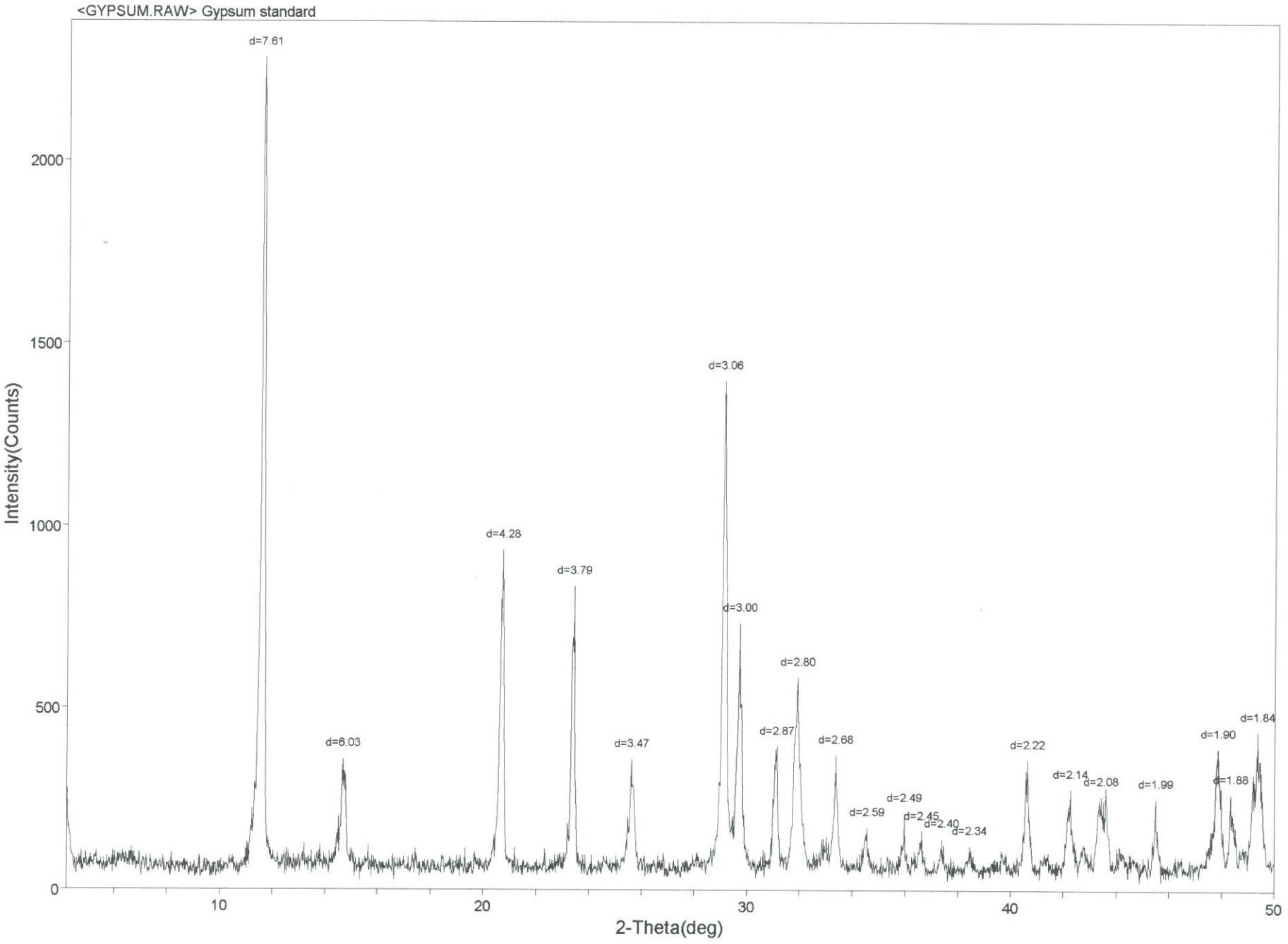

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Appendix 3.

X-ray diffraction peaks used to identify minerals present in bulk samples

Appendix 3. X-ray diffraction peaks used to identify minerals present in bulk samples.

14.00	Smectite or chlorite
14-10	Mixed-layer clays
10.00	Illite
7.61	Gypsum
7.14	Kaolinite
6.03	Gypsum
4.48	Kaolinite
4.28	Gypsum
4.26	Quartz
3.86	Calcite
3.80	Gypsum
3.58	Kaolinite
3.47	Gypsum
3.34	Quartz
3.33	Illite
3.29-3.24	Orthoclase
3.18	Plagioclase
3.07	Gypsum
3.04	Calcite
3.00	Gypsum
2.88	Dolomite
2.67	Dolomite
2.57	Kaolinite
2.50	Kaolinite
2.50	Calcite
2.46	Quartz
2.39	Kaolinite
2.34	Kaolinite
2.29	Calcite
2.28	Quartz
2.24	Quartz
2.19	Dolomite
2.13	Quartz
2.10	Calcite
2.01	Illite
1.99	Kaolinite
1.98	Quartz
1.91	Calcite
1.88	Calcite
1.82	Quartz

Notes: Not all of the peaks listed in the ASTM data file of x-ray diffraction peaks were observed for these minerals. Except for quartz, most were present in too small amounts for

any peaks except for those of high intensity to appear.

Not all peaks appear at their ideal position. In mixtures of several minerals such as these samples, interference of peaks from different minerals can cause the resulting peak to shift. Also, it is difficult to determine exactly the position of the top of a peak when the peaks are of low intensity such as most of the peaks that appear on these samples.

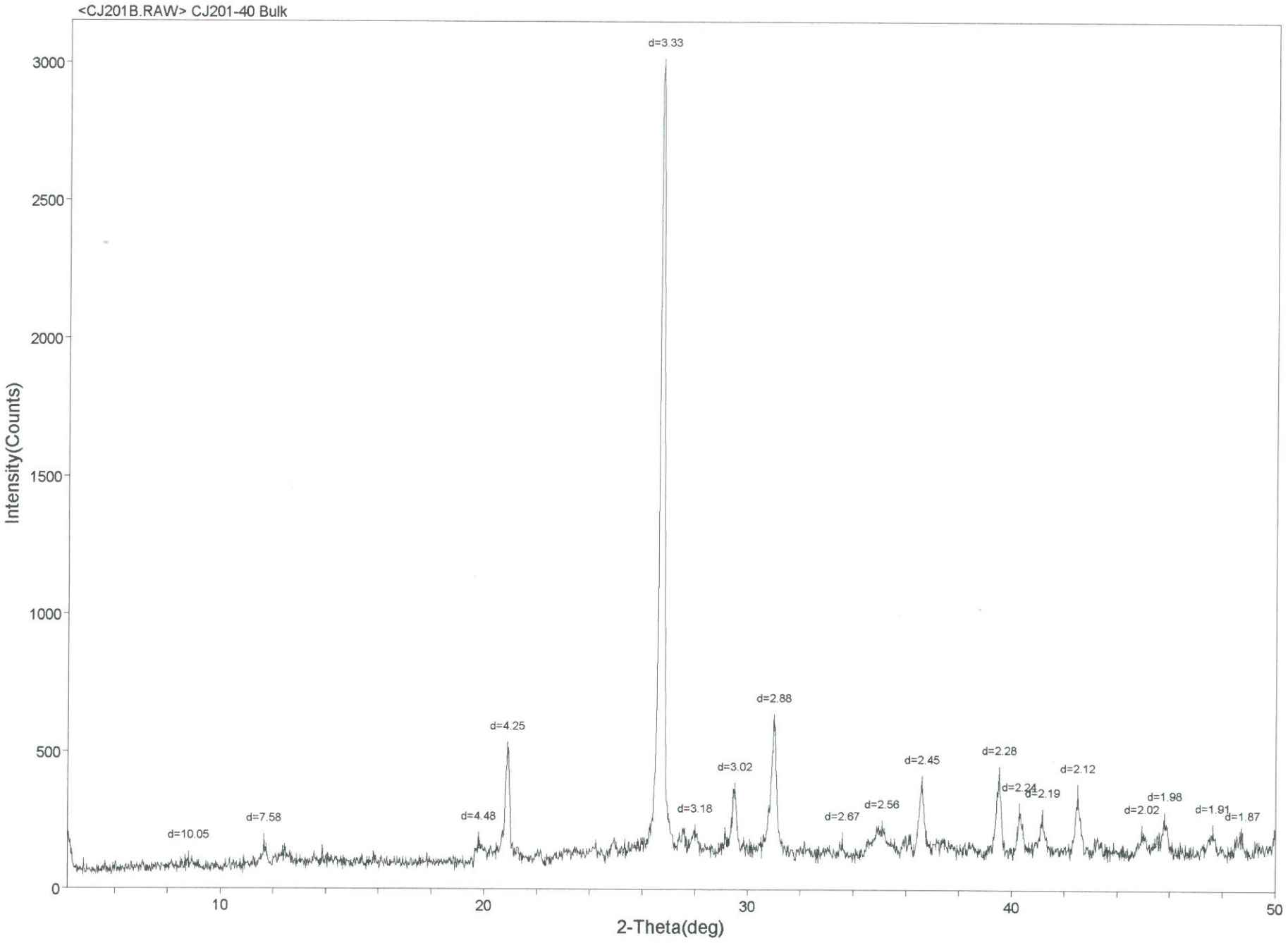
Appendix 4.

X-ray diffraction patterns of bulk samples

Appendix 4. X-ray diffraction patterns of bulk samples.

Two copies of each diffraction pattern are presented. The first of each pair is annotated with the d-spacings of most diffraction peaks. A few were not annotated because the closeness of other peaks would make the annotations unreadable.

The second of each pair is annotated with letters showing the identities of the most intense peaks. Not all of the minor peaks were annotated, although they were accounted for.



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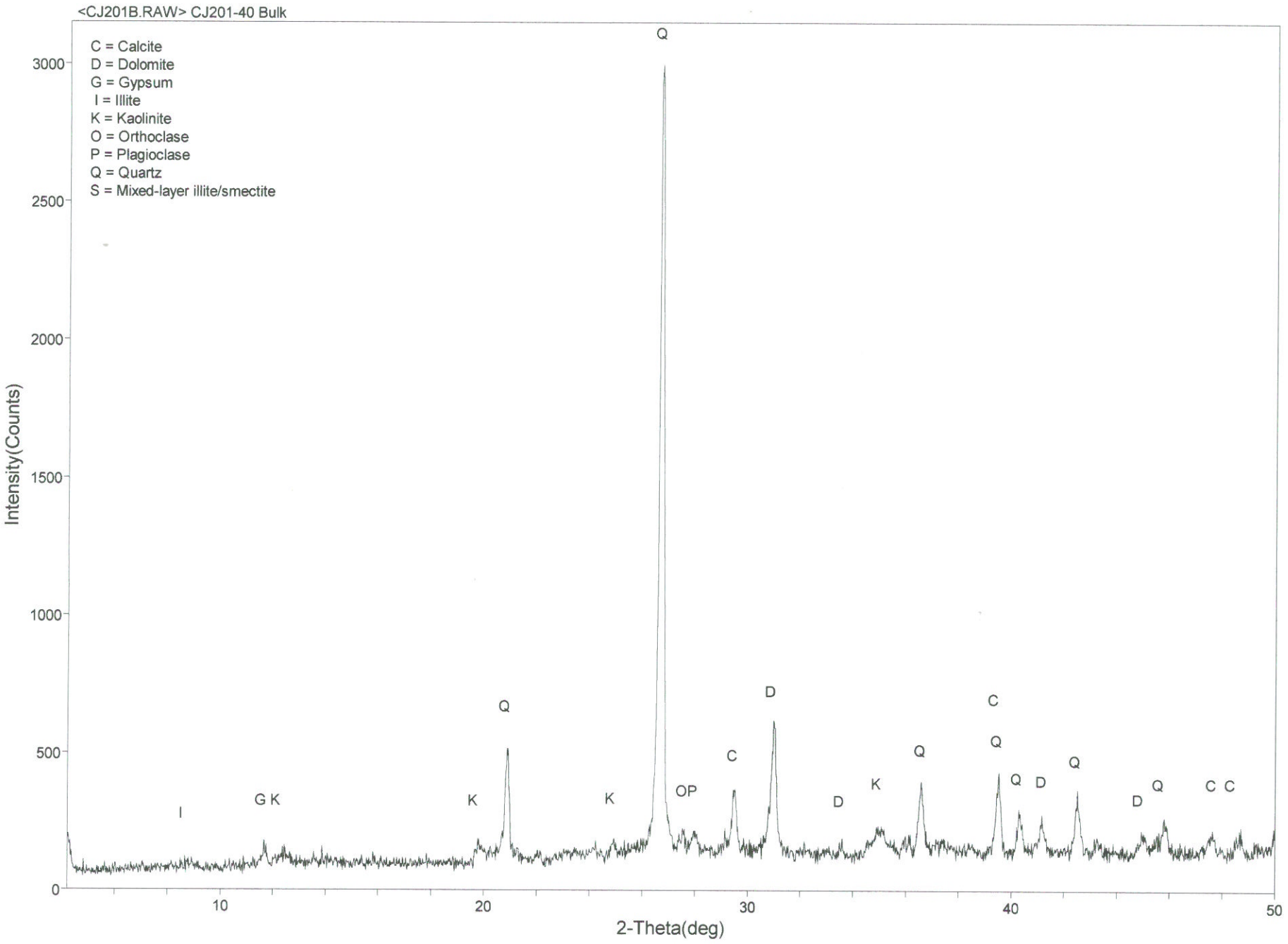

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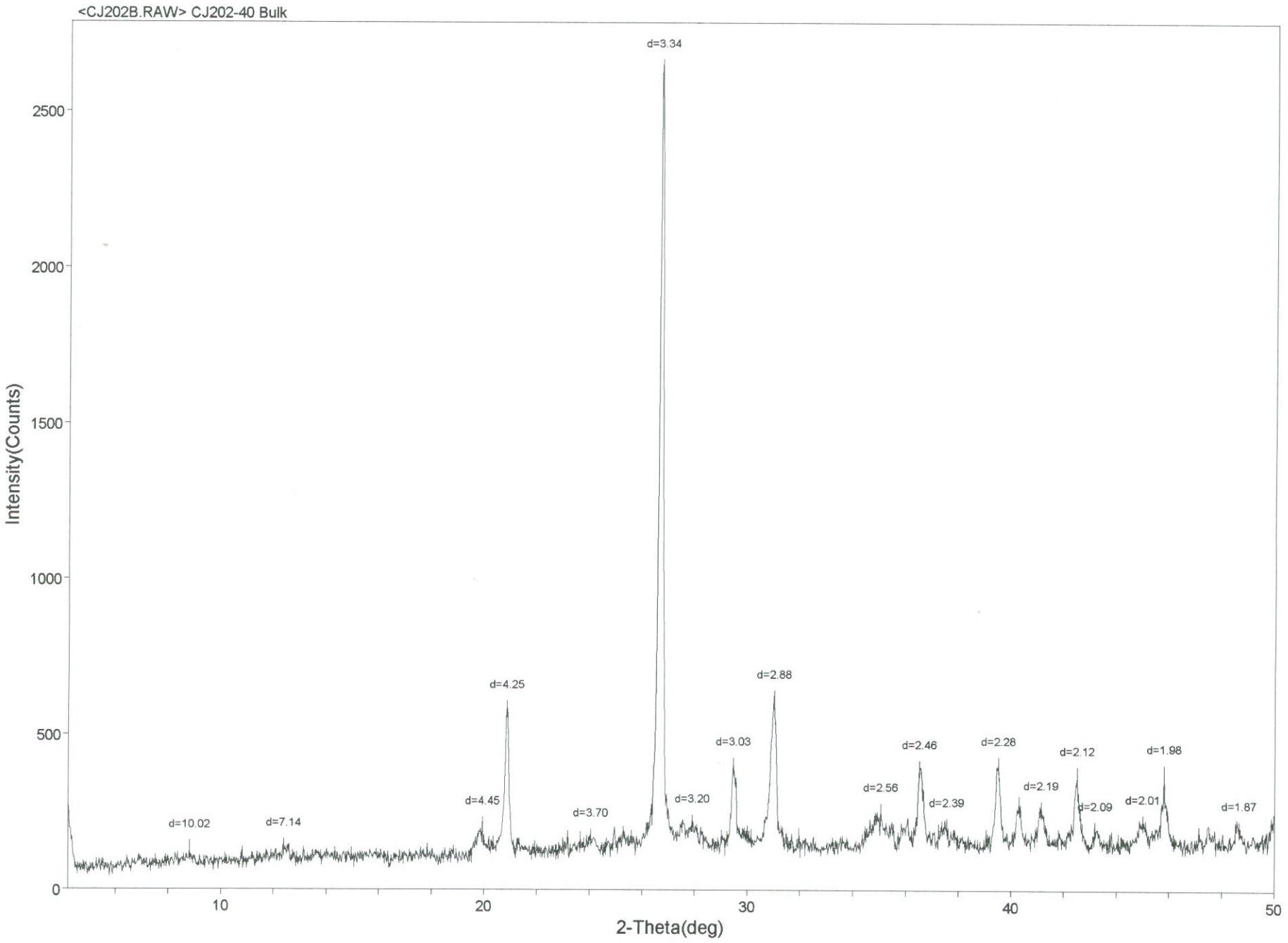

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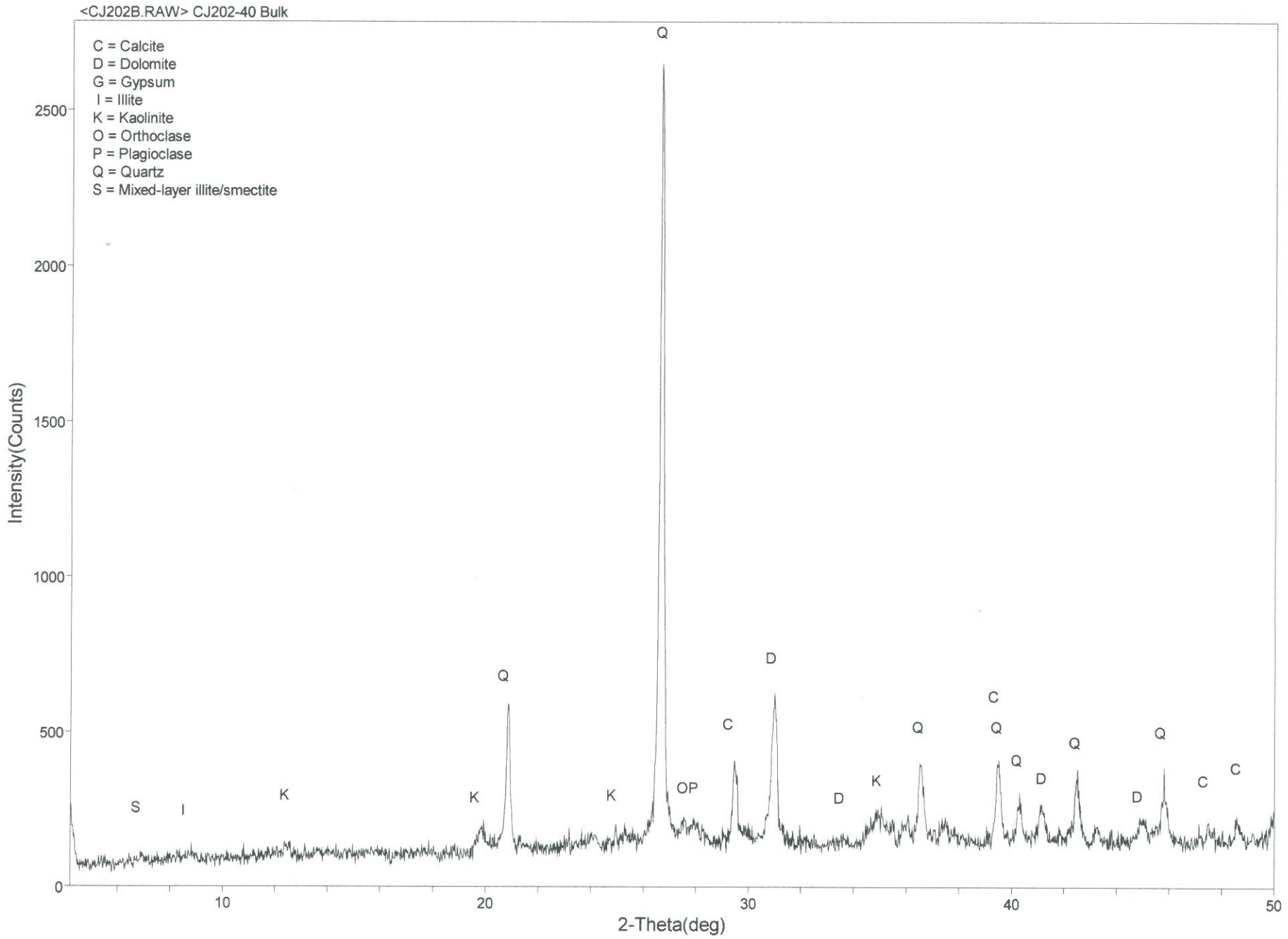

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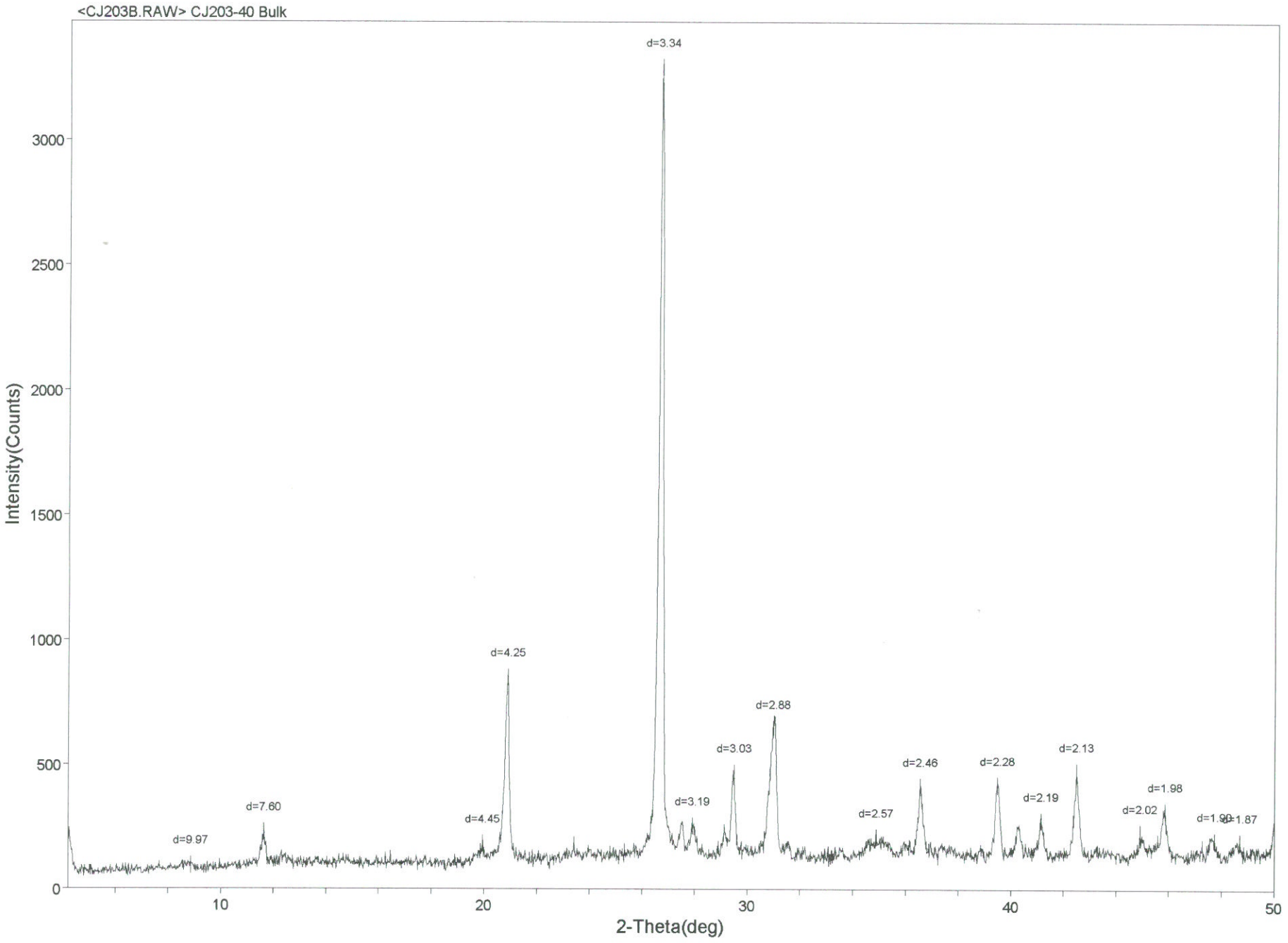

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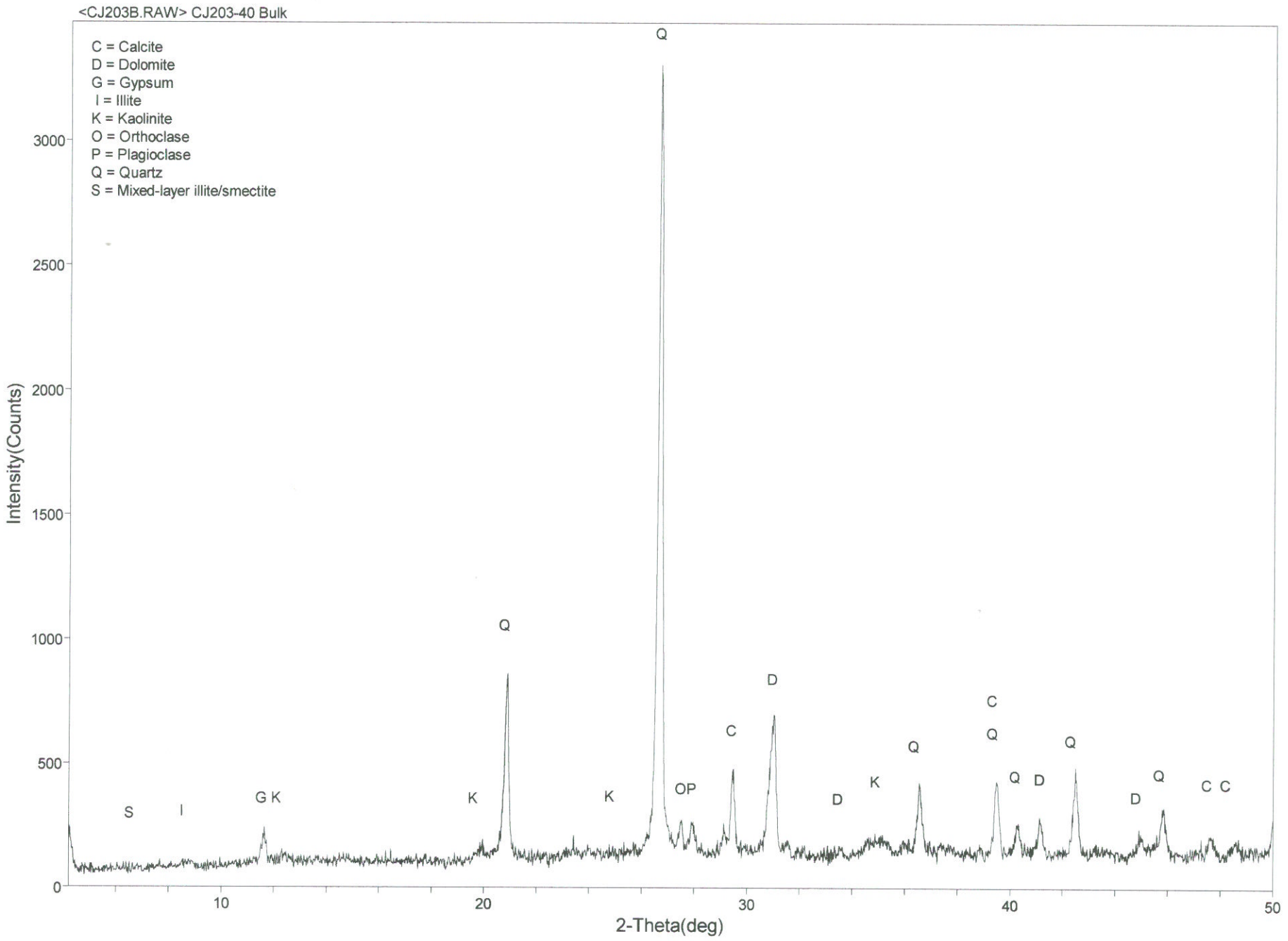

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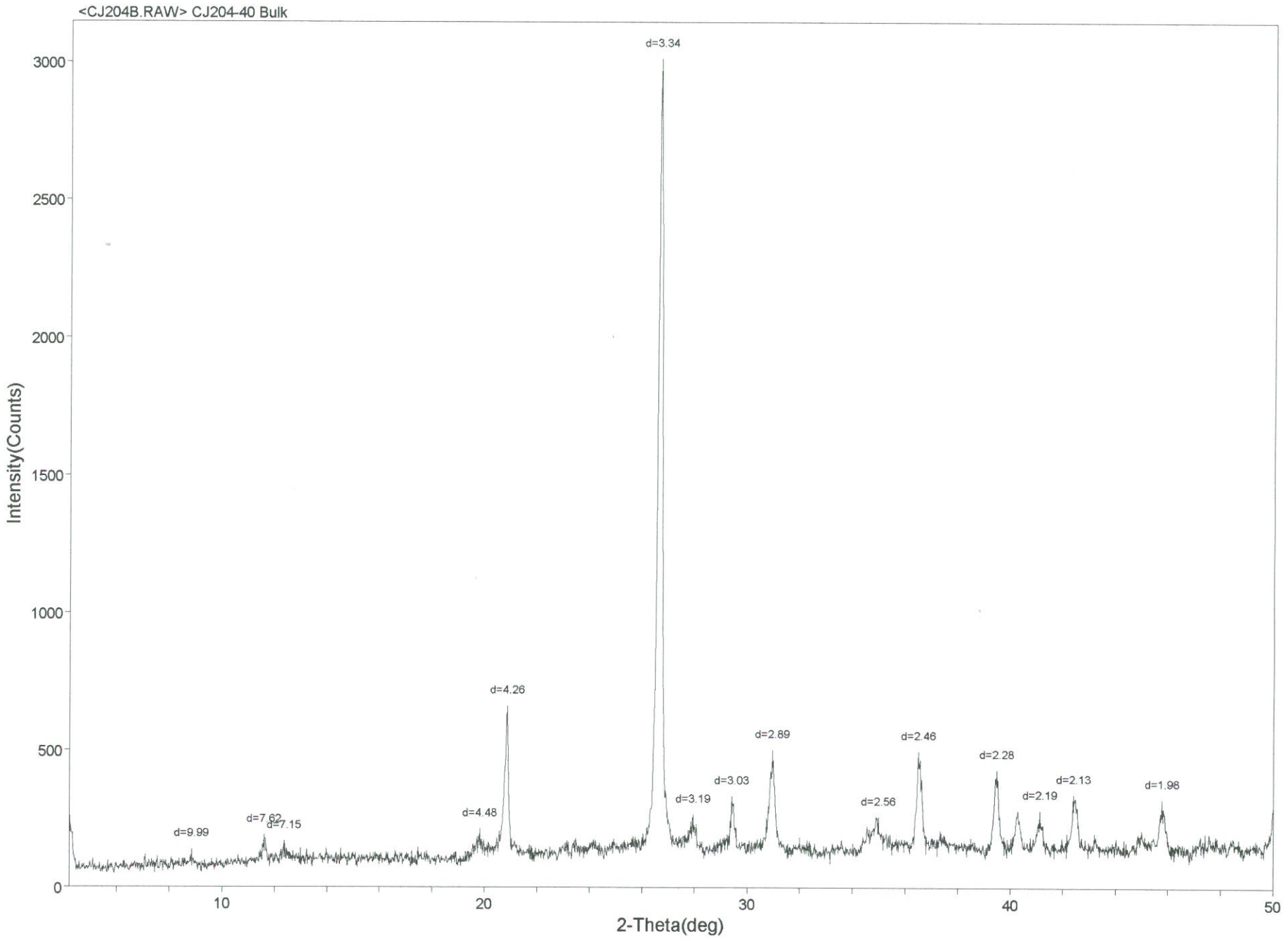

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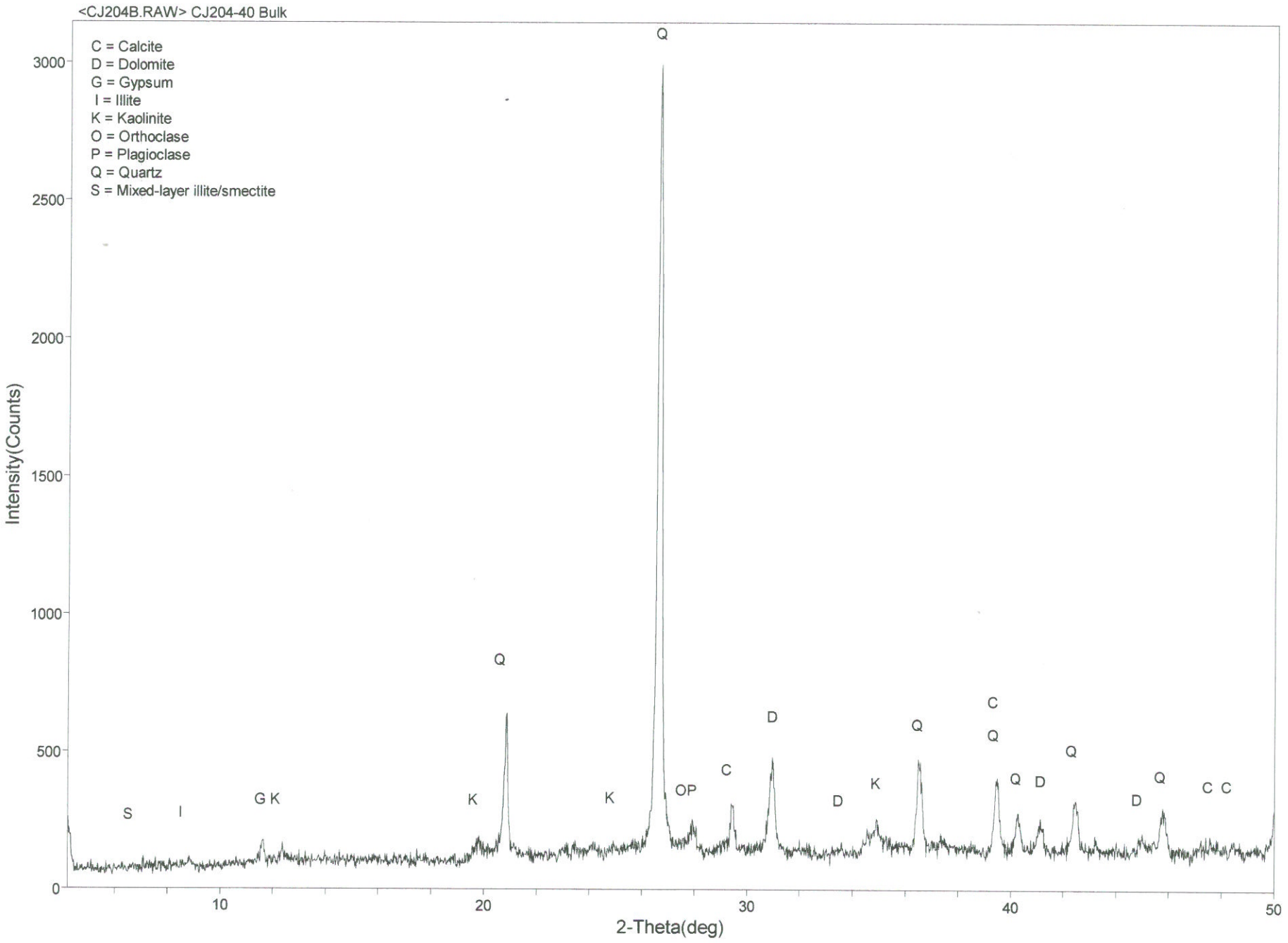

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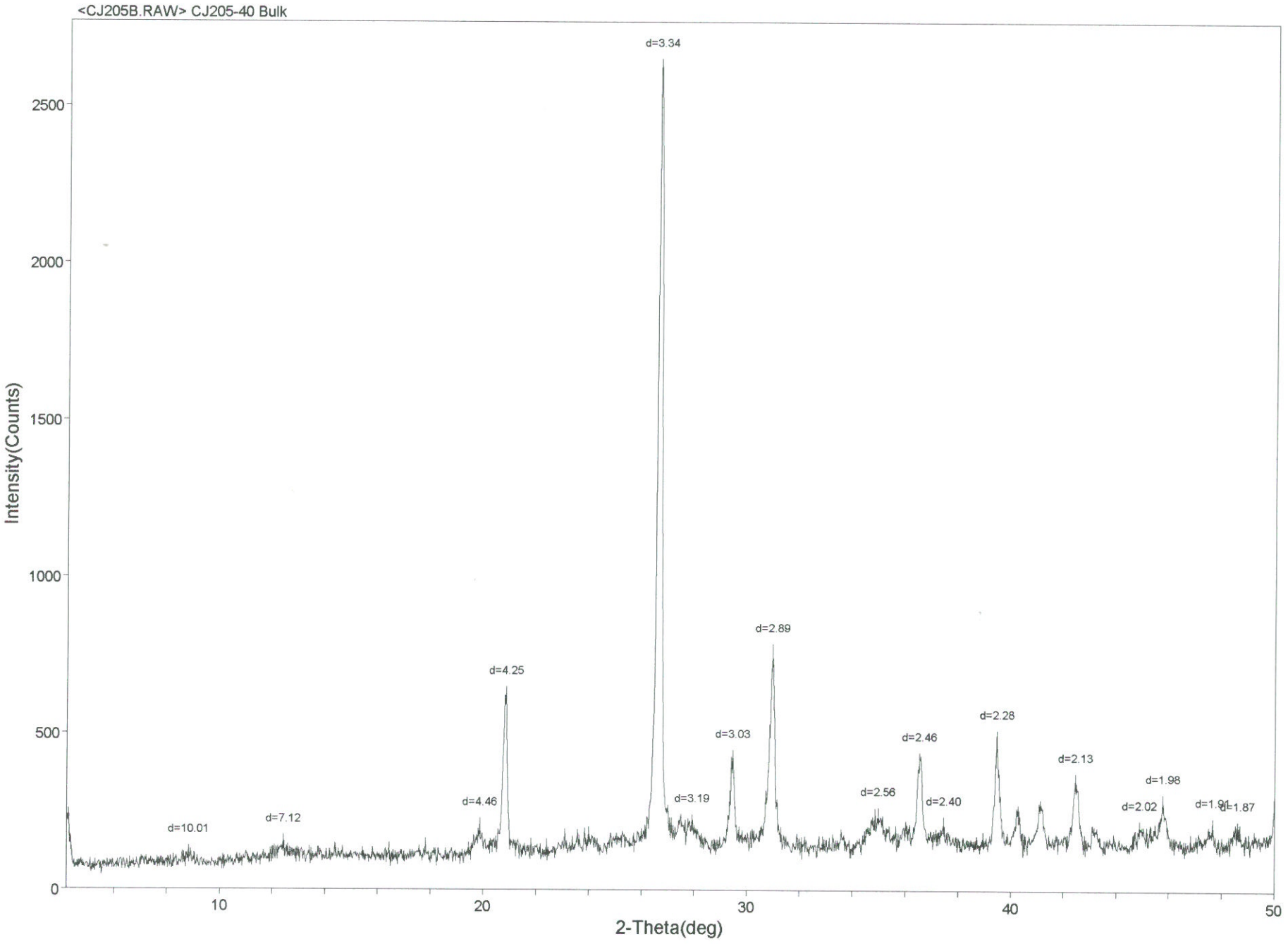

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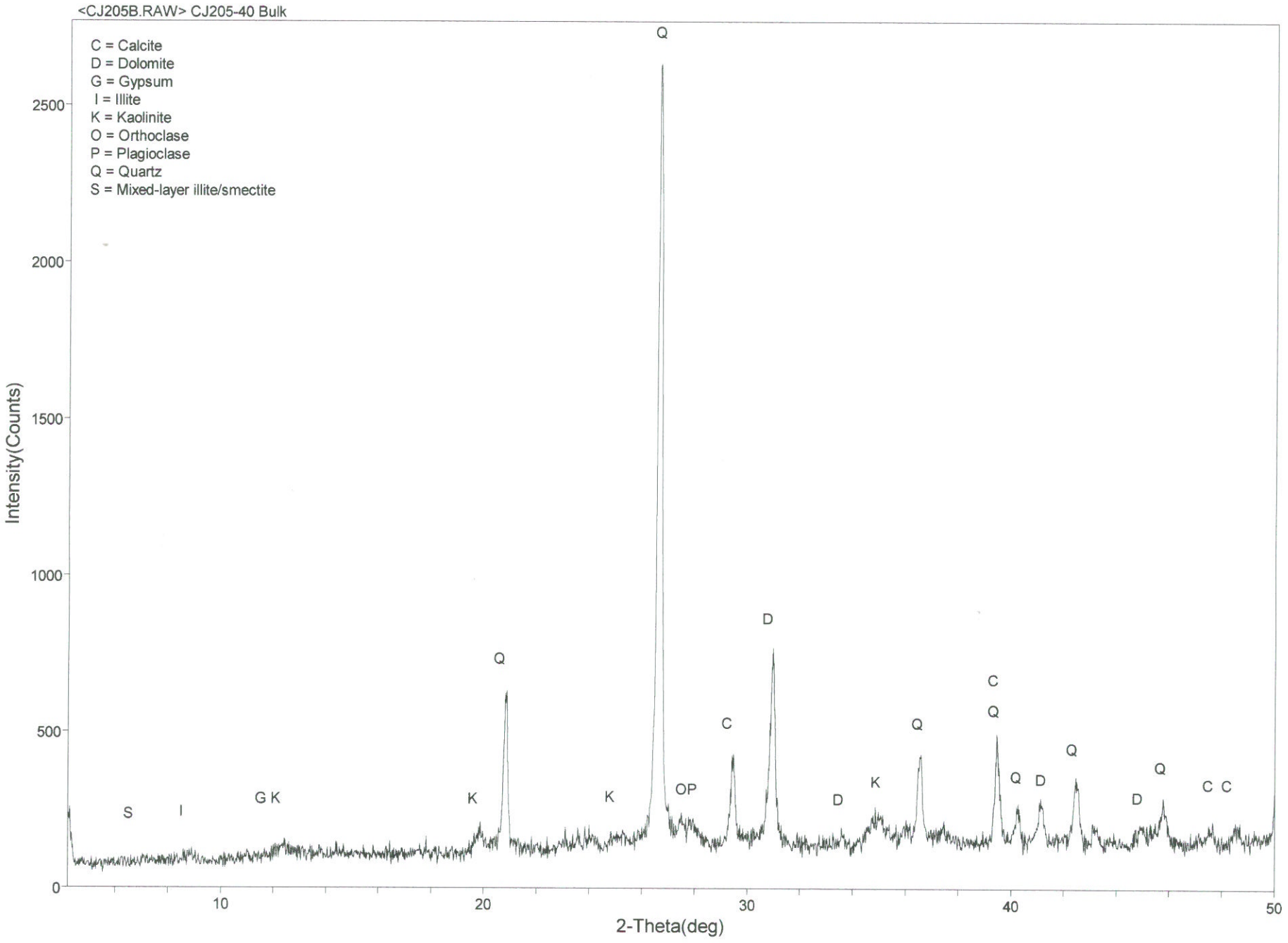

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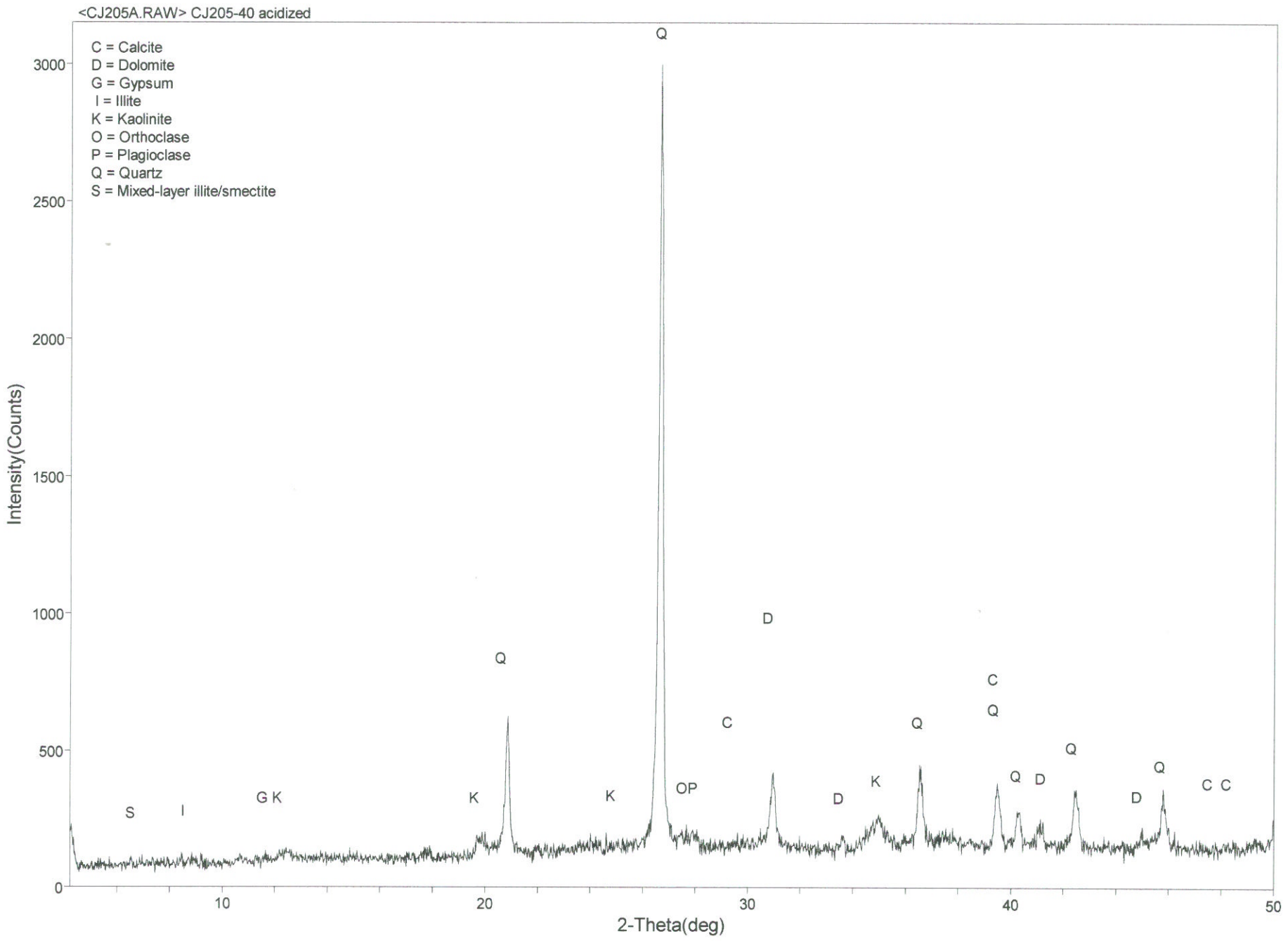

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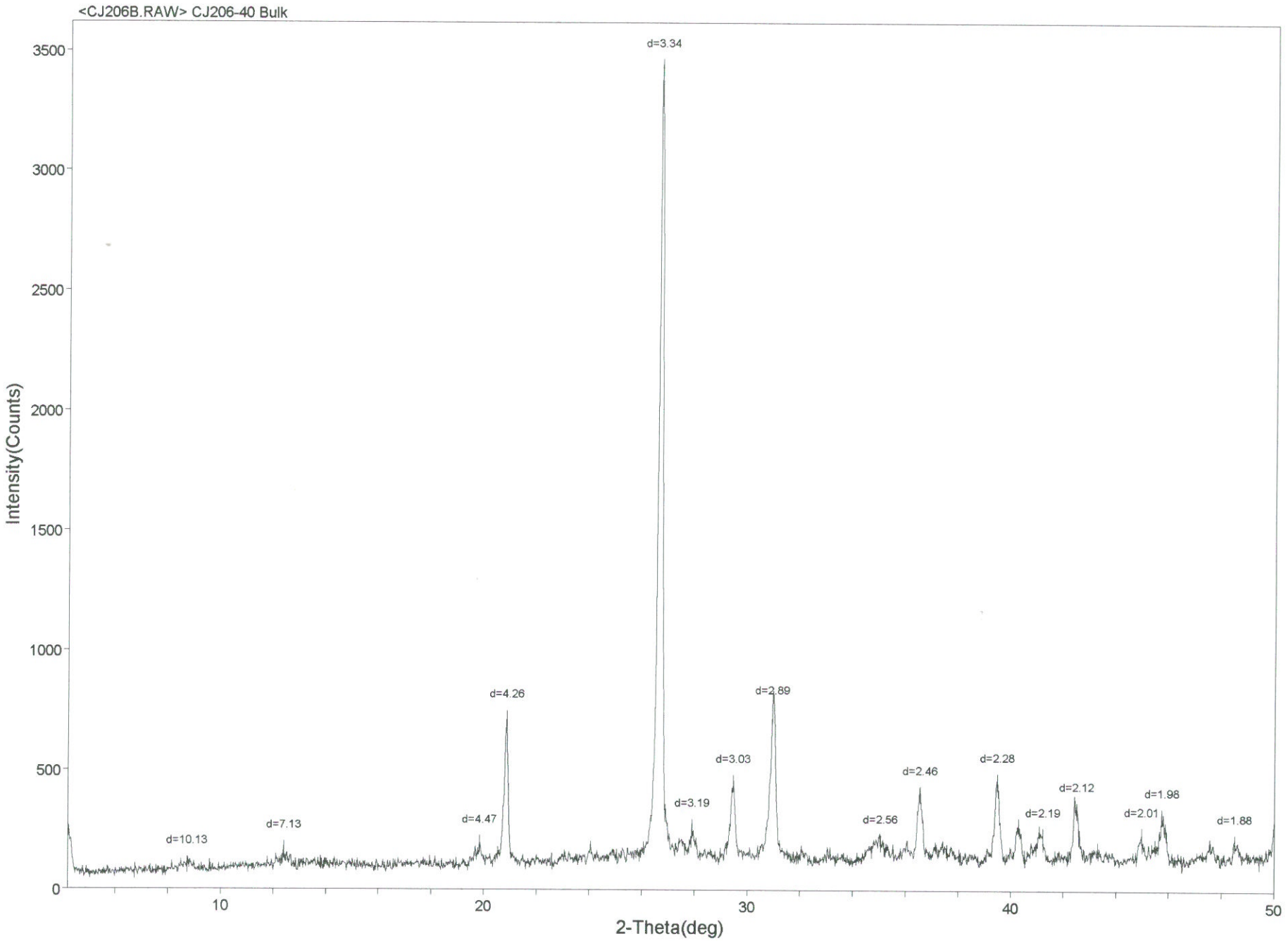

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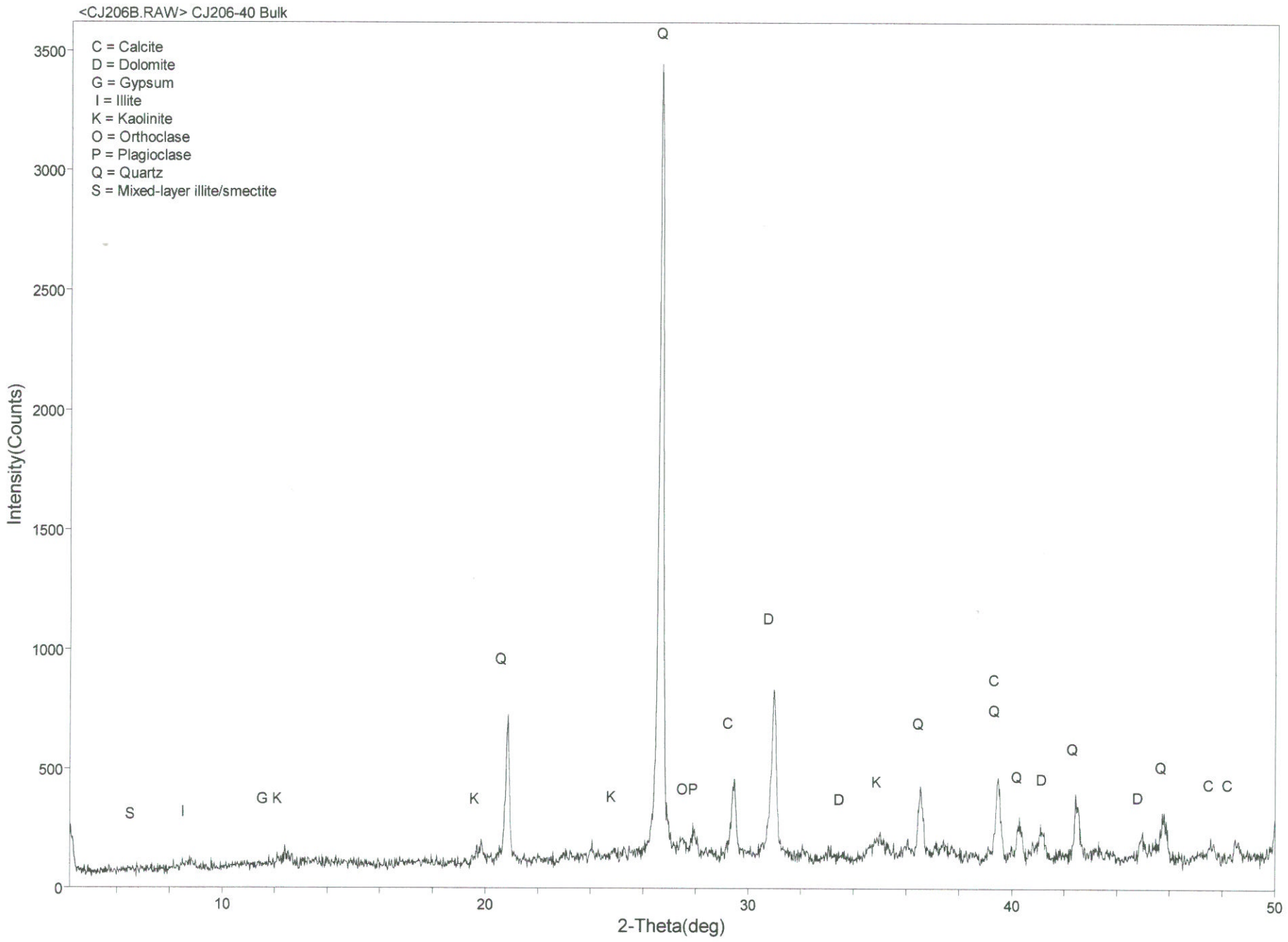

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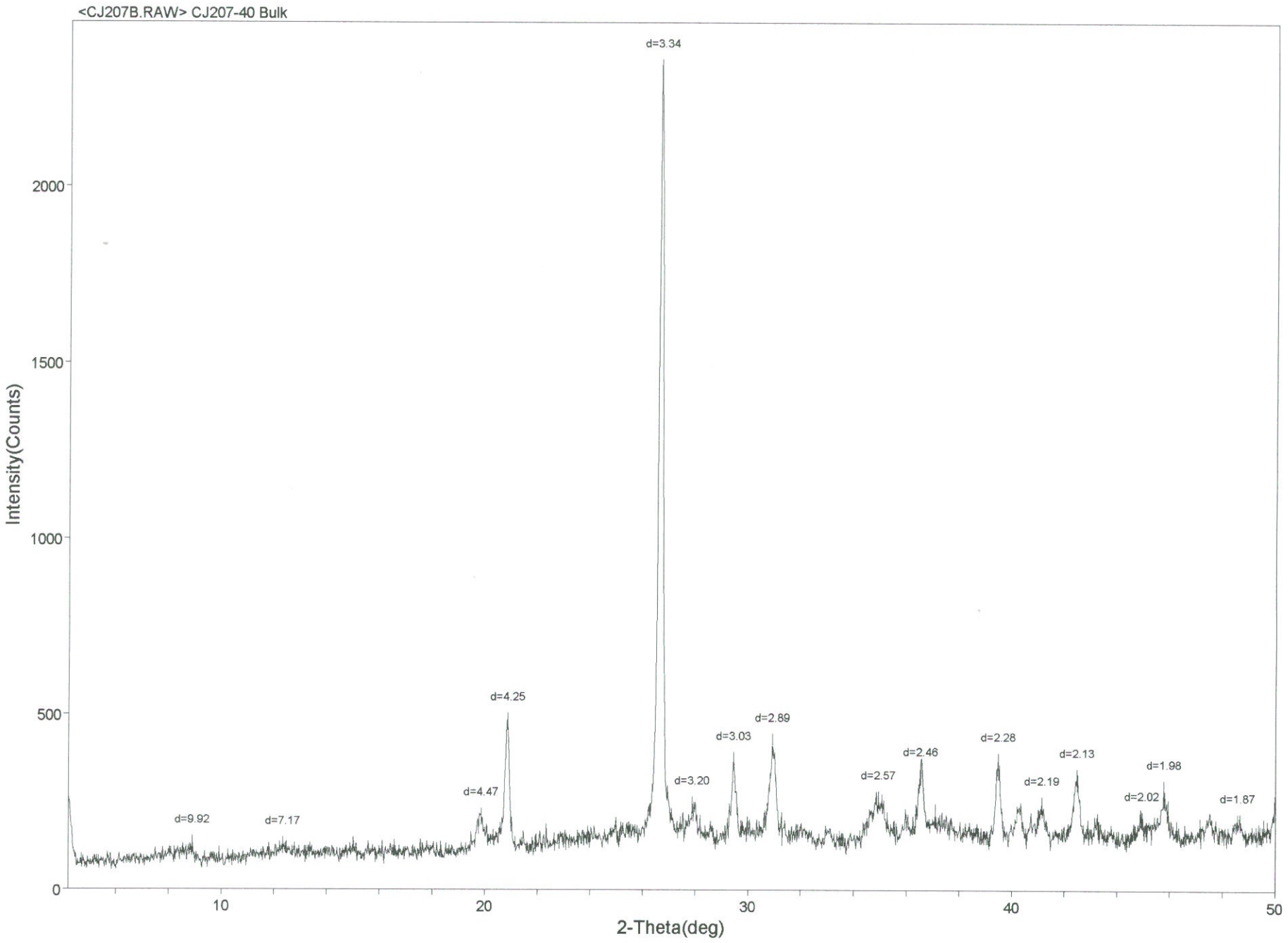

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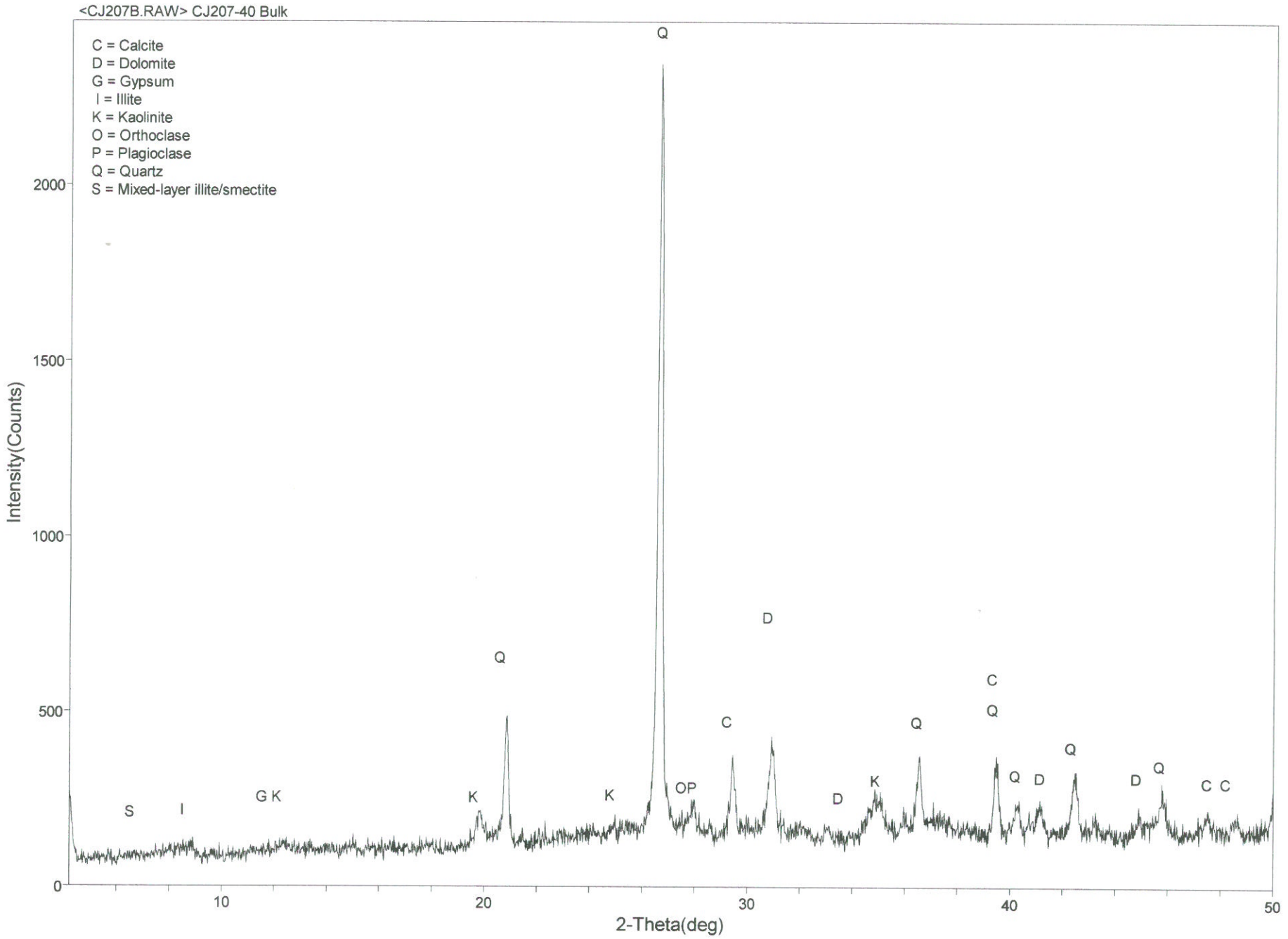

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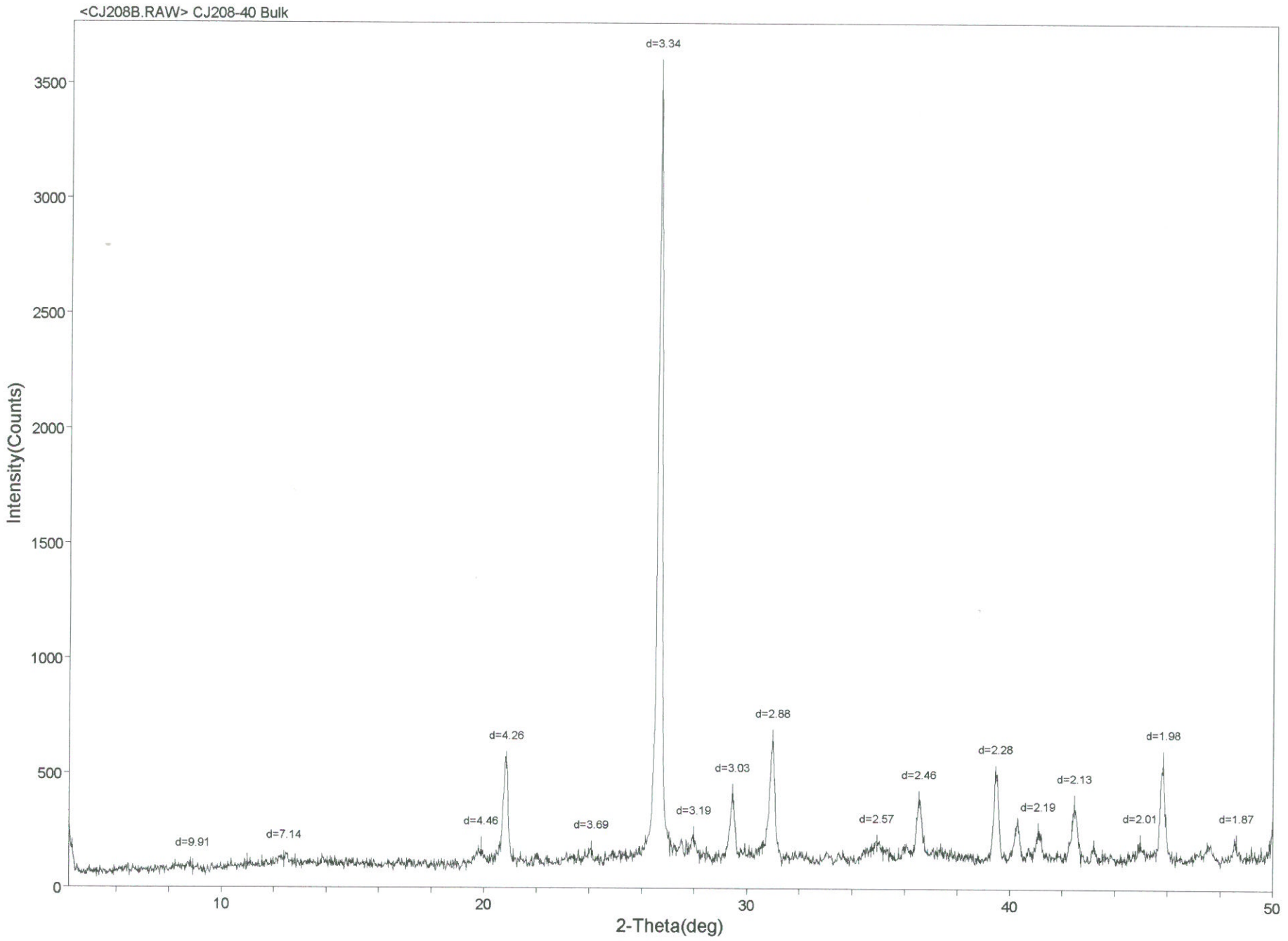

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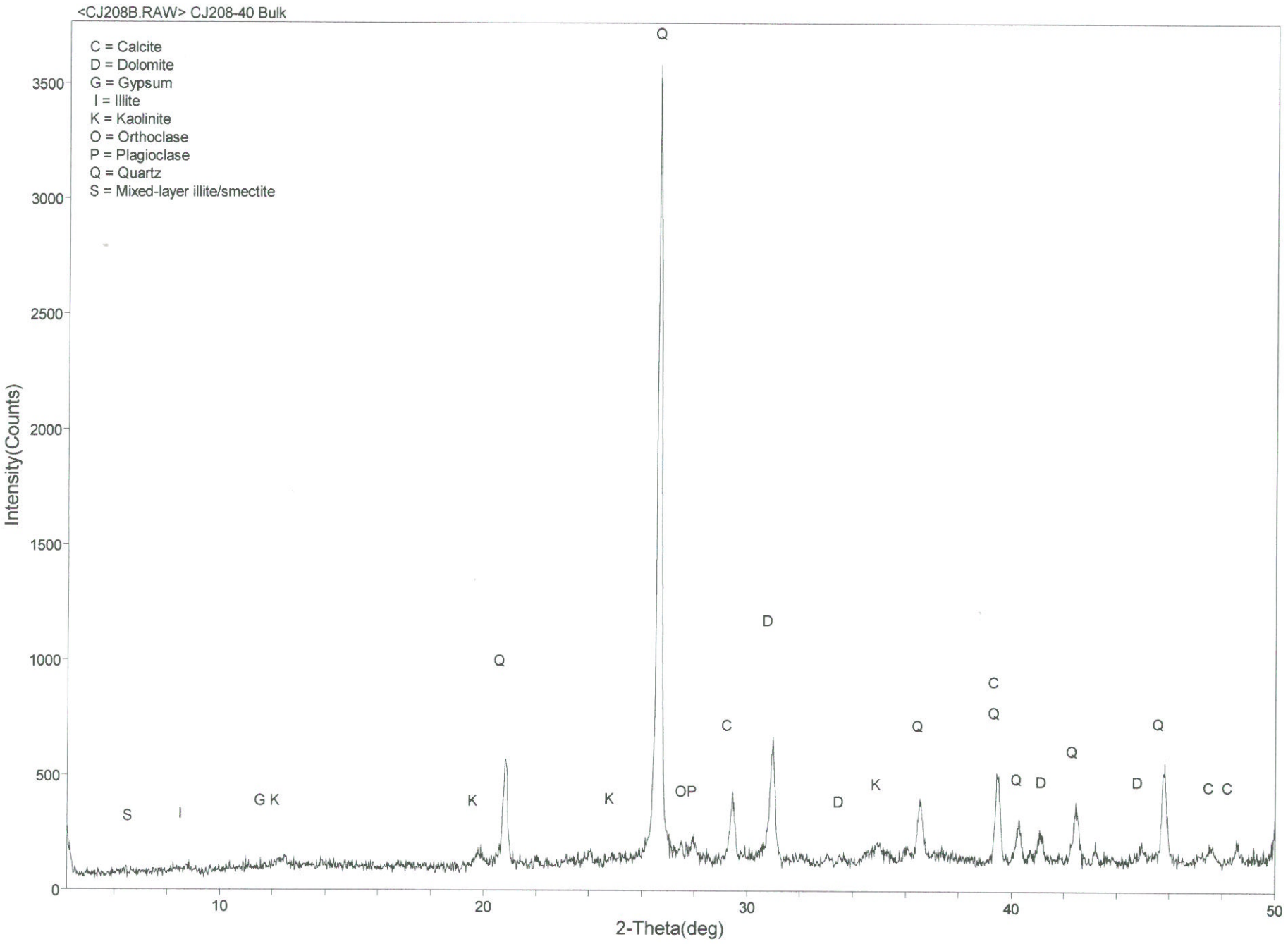

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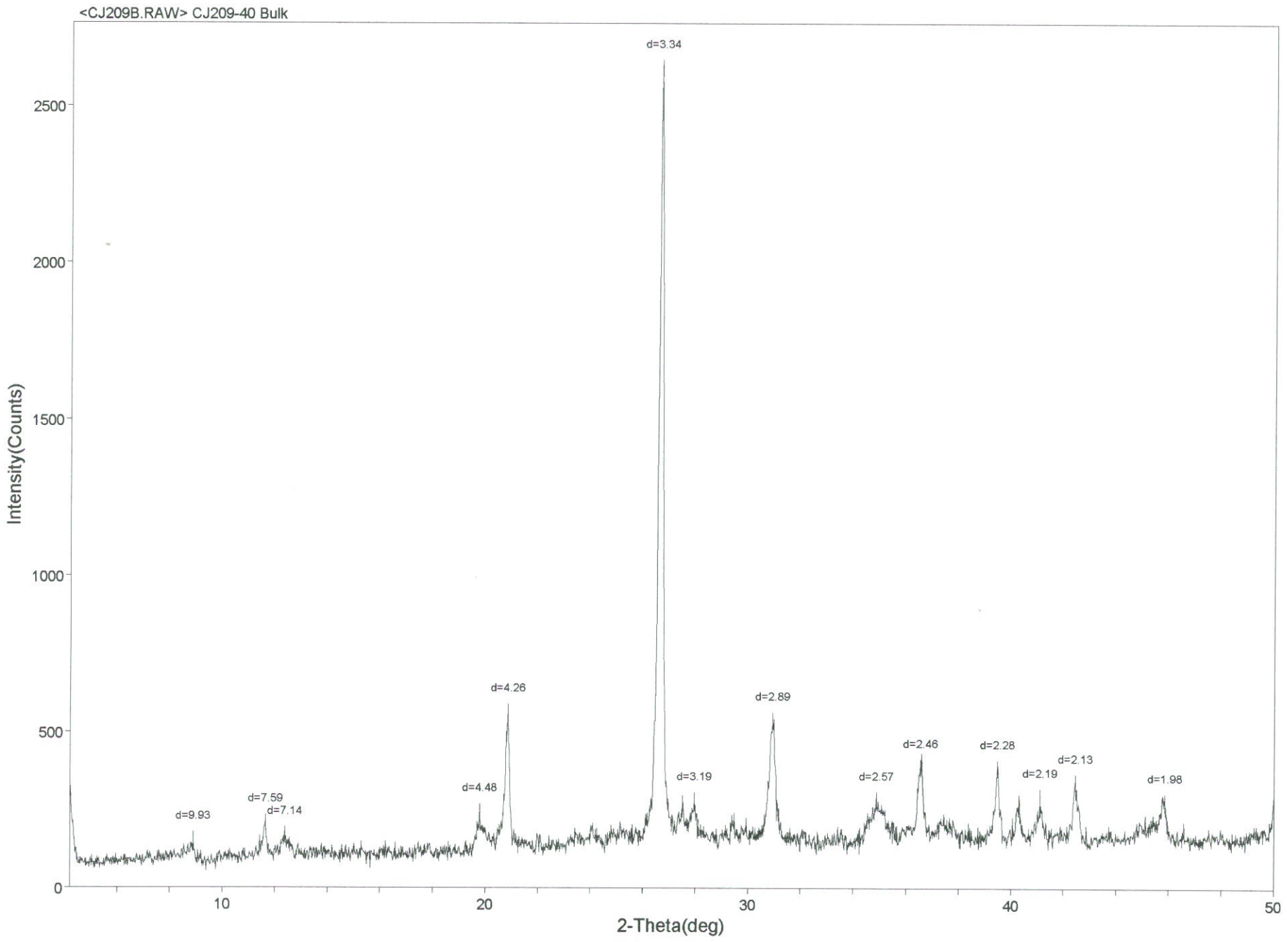

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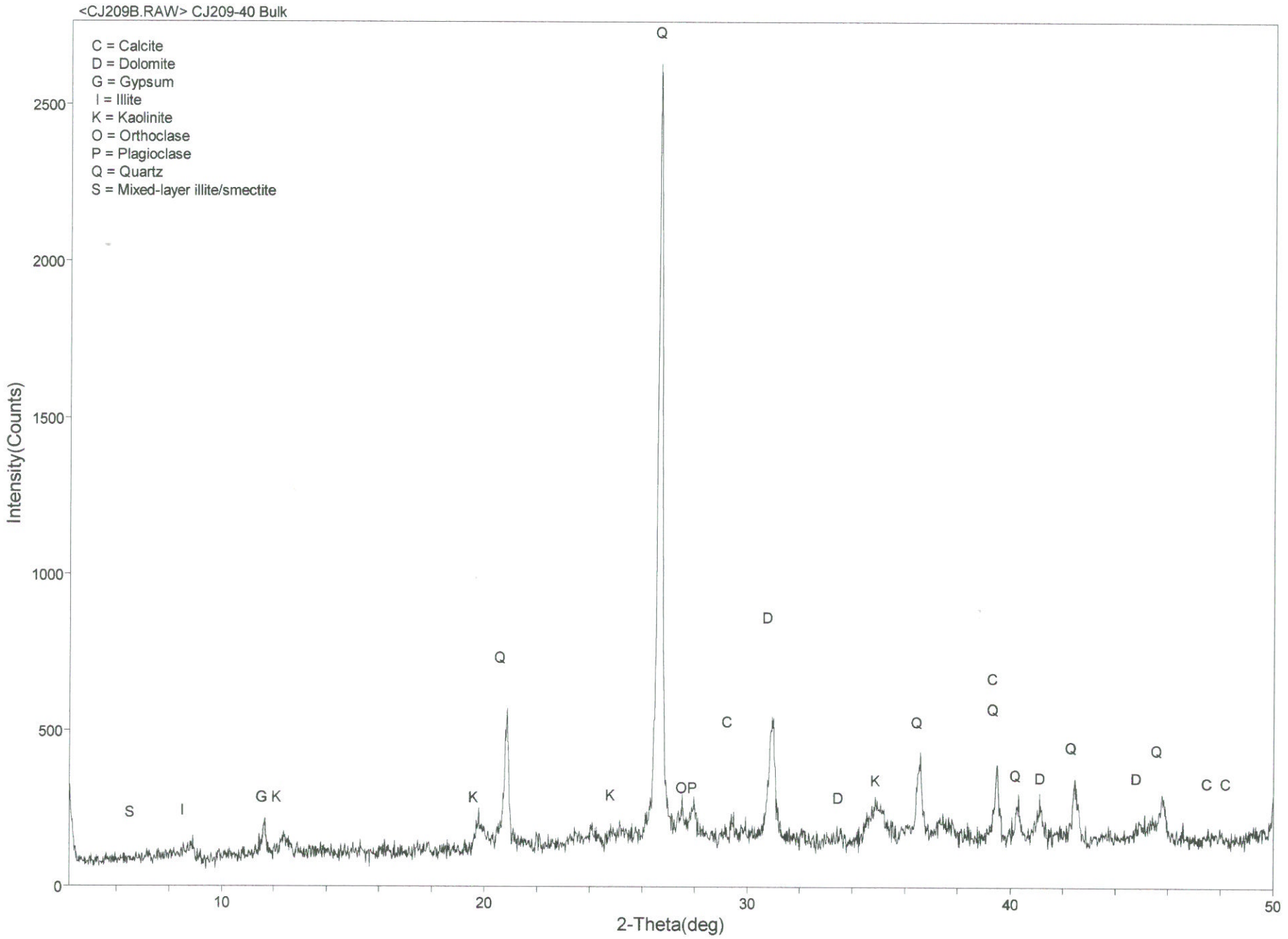

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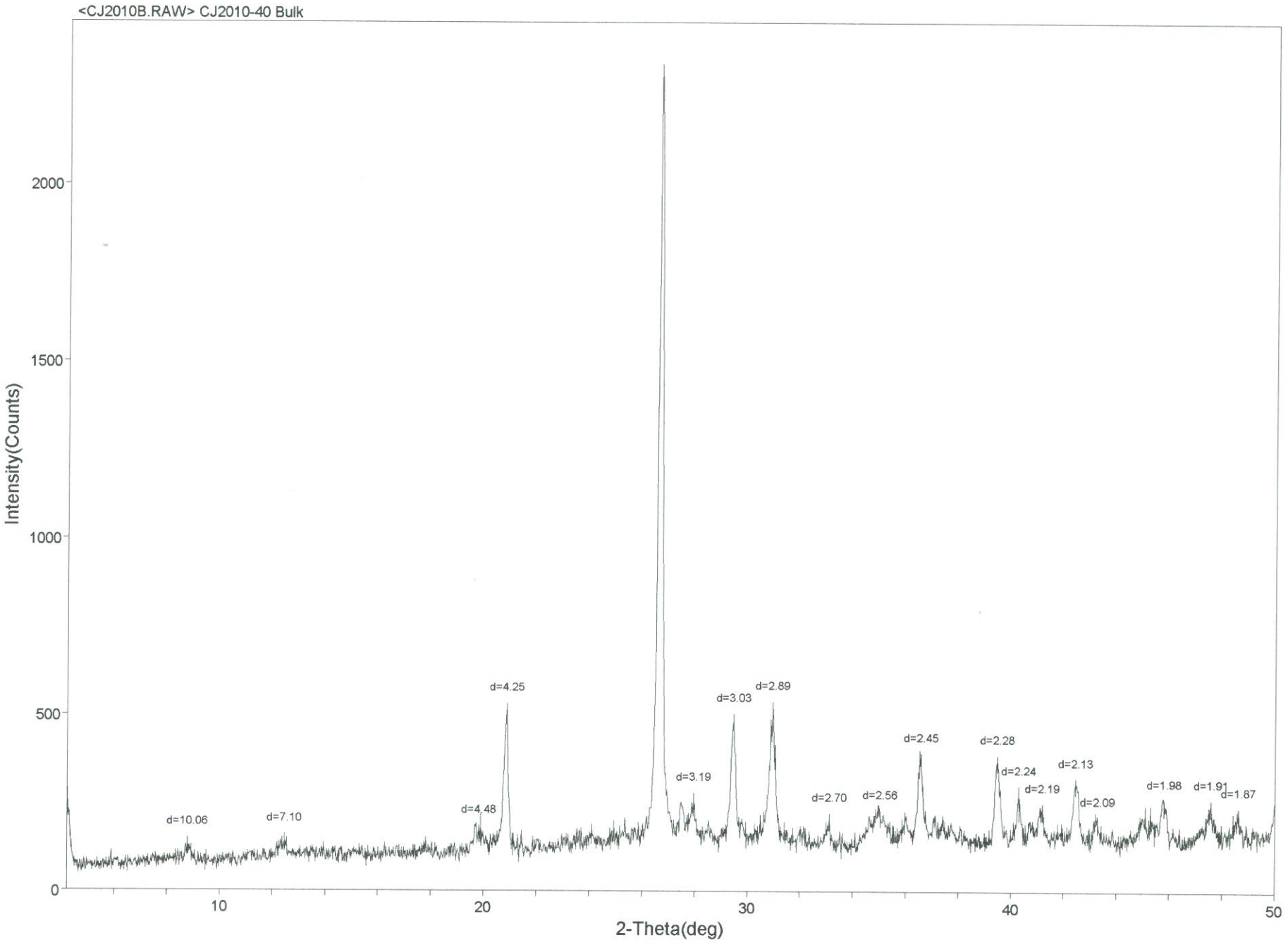

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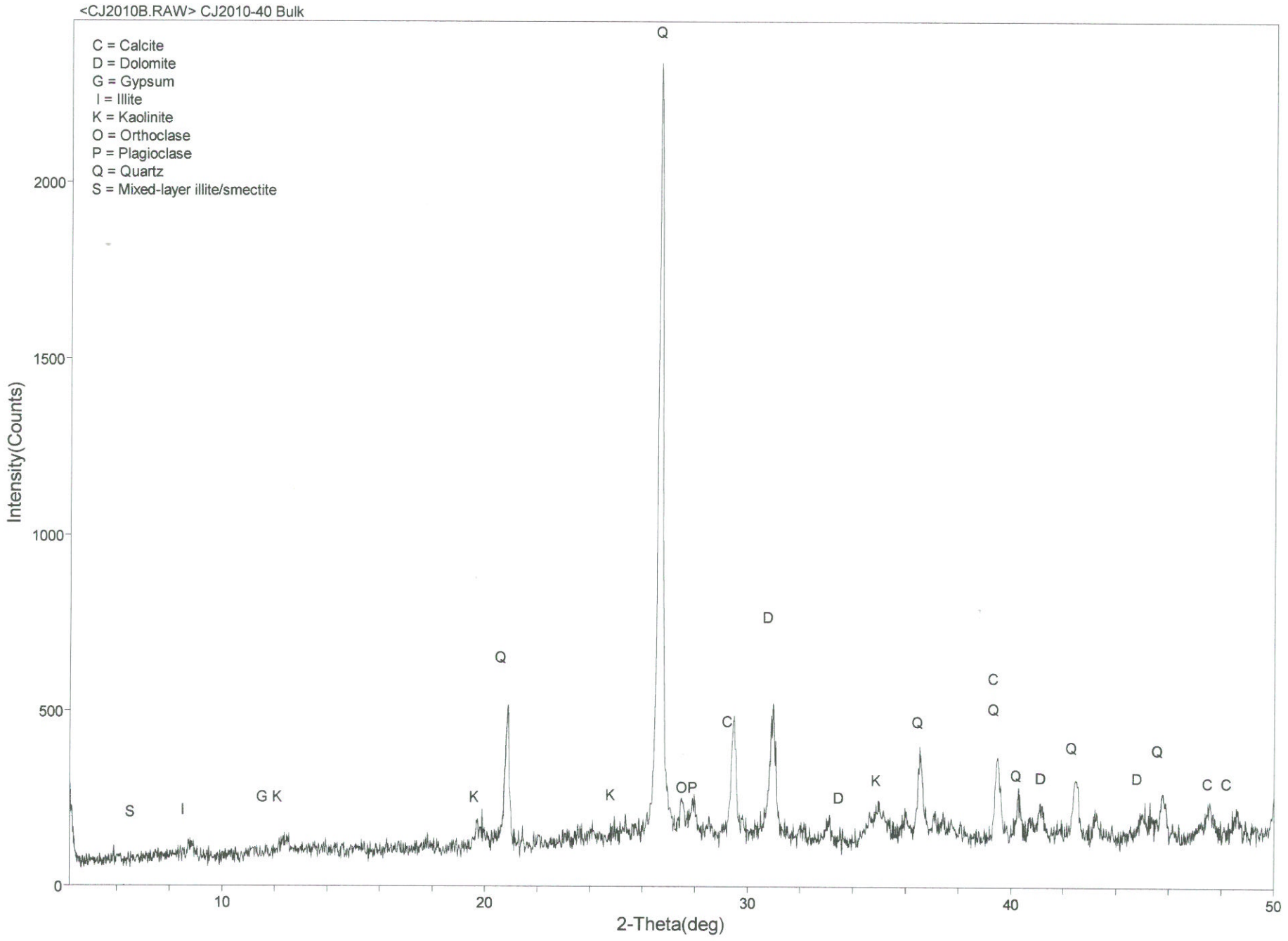

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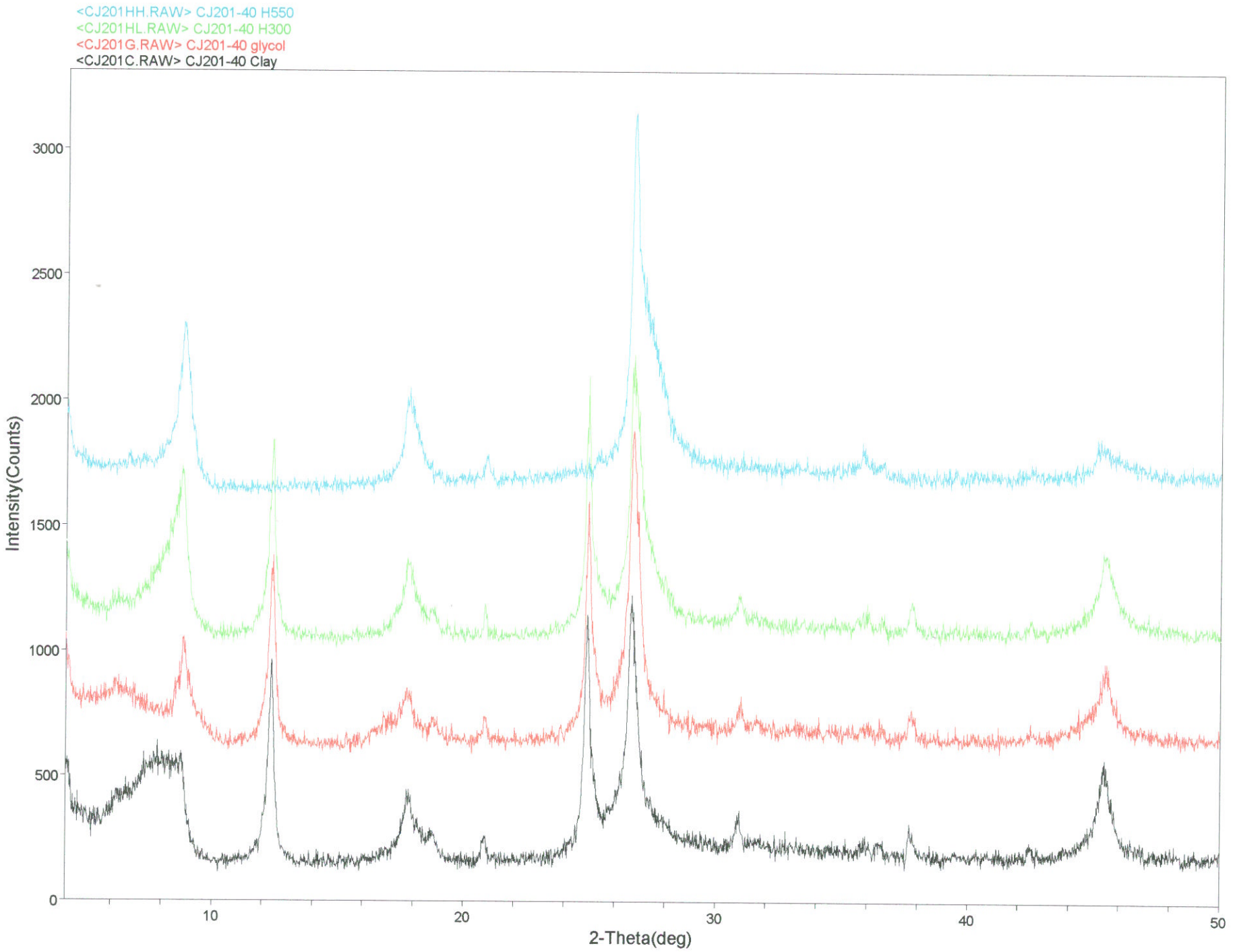
Appendix 5.

Stacked x-ray diffraction patterns of clay minerals in CJ sample set



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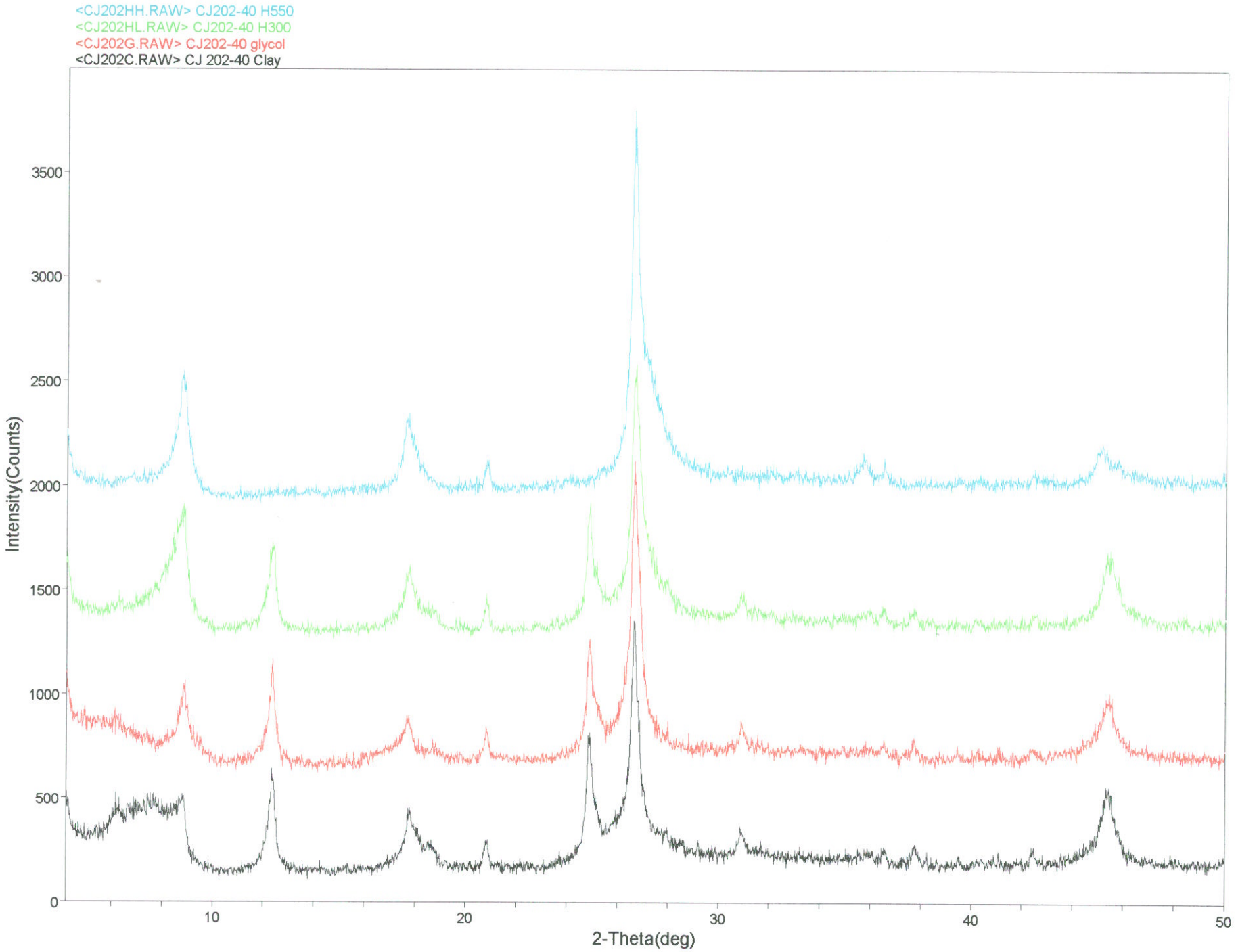

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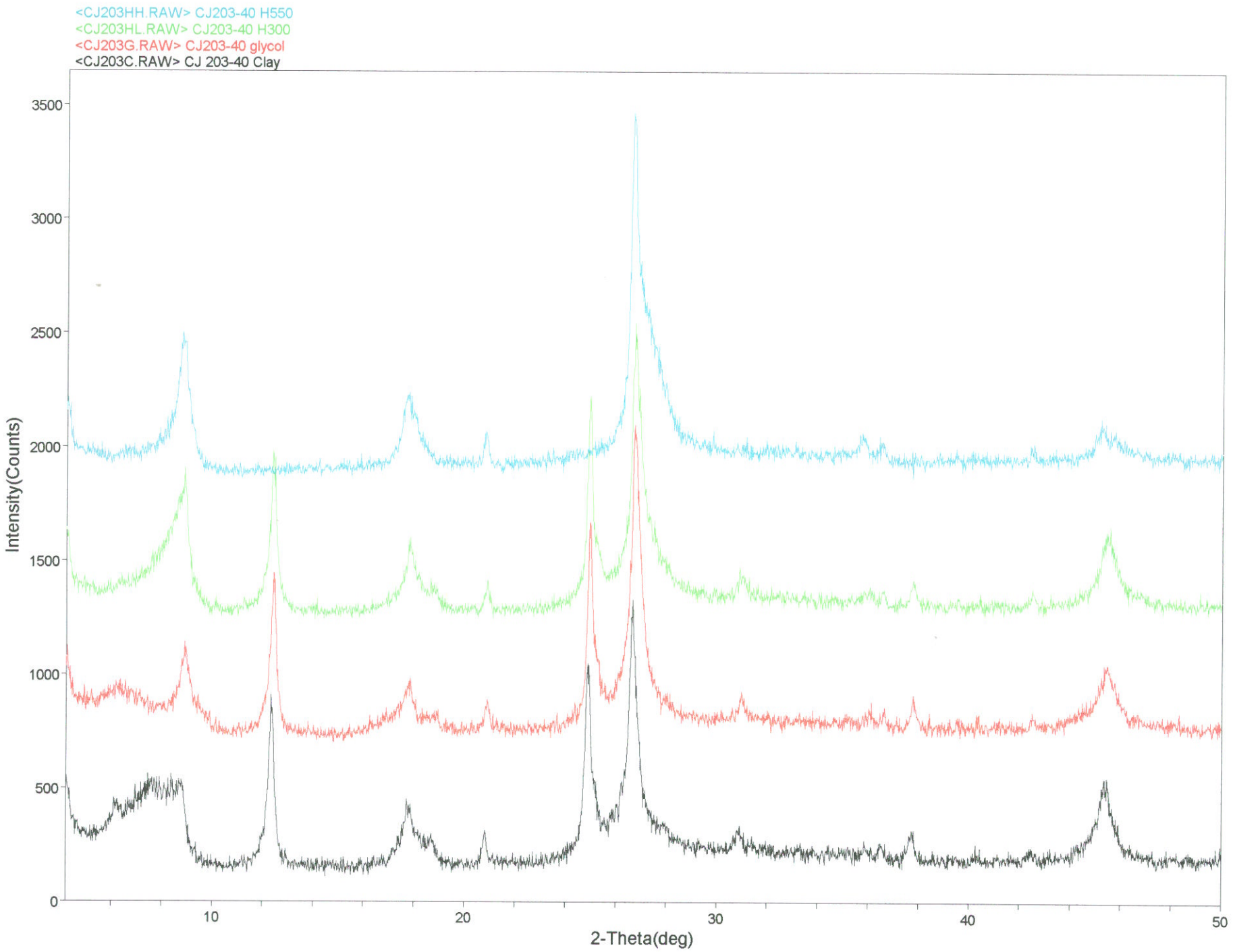

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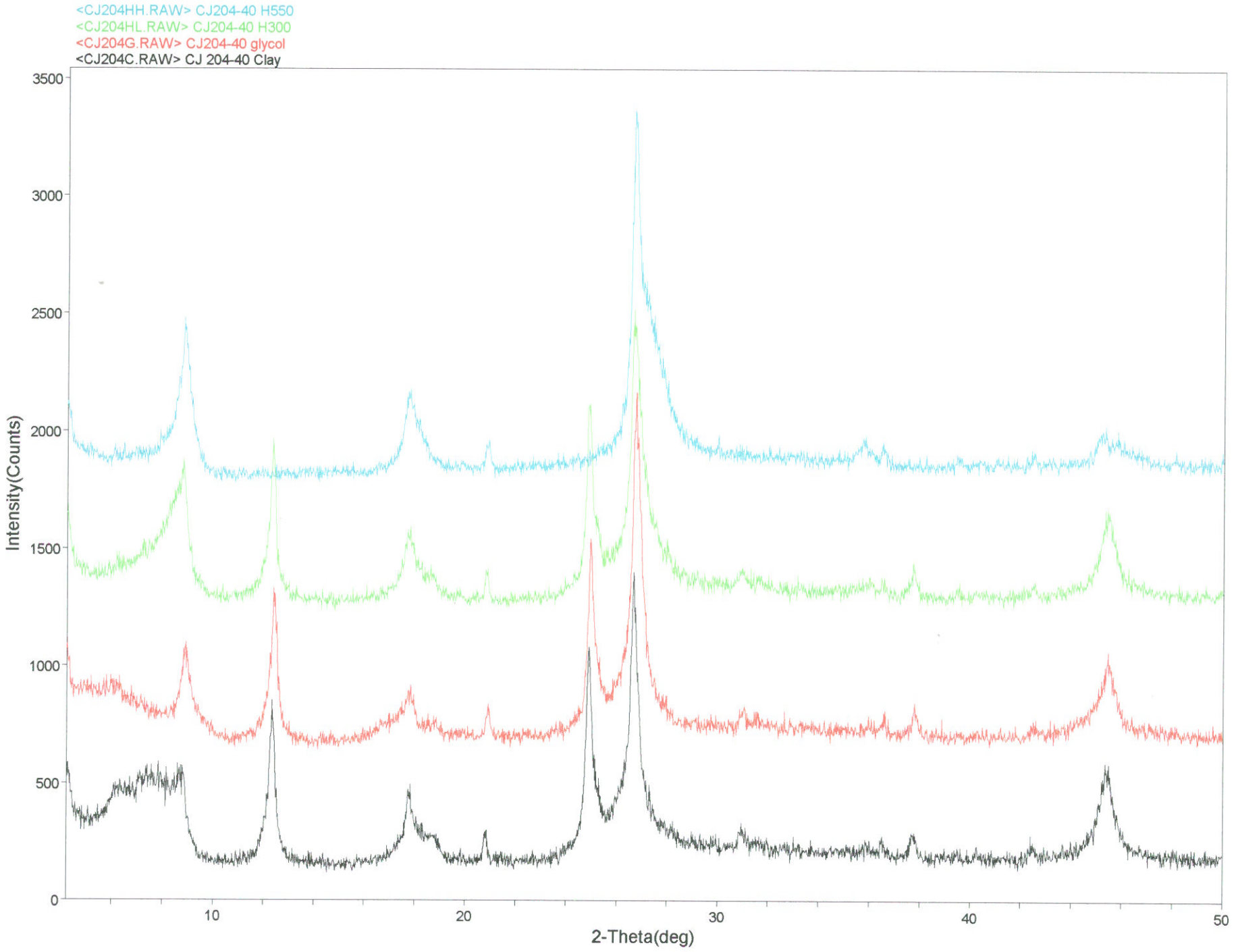

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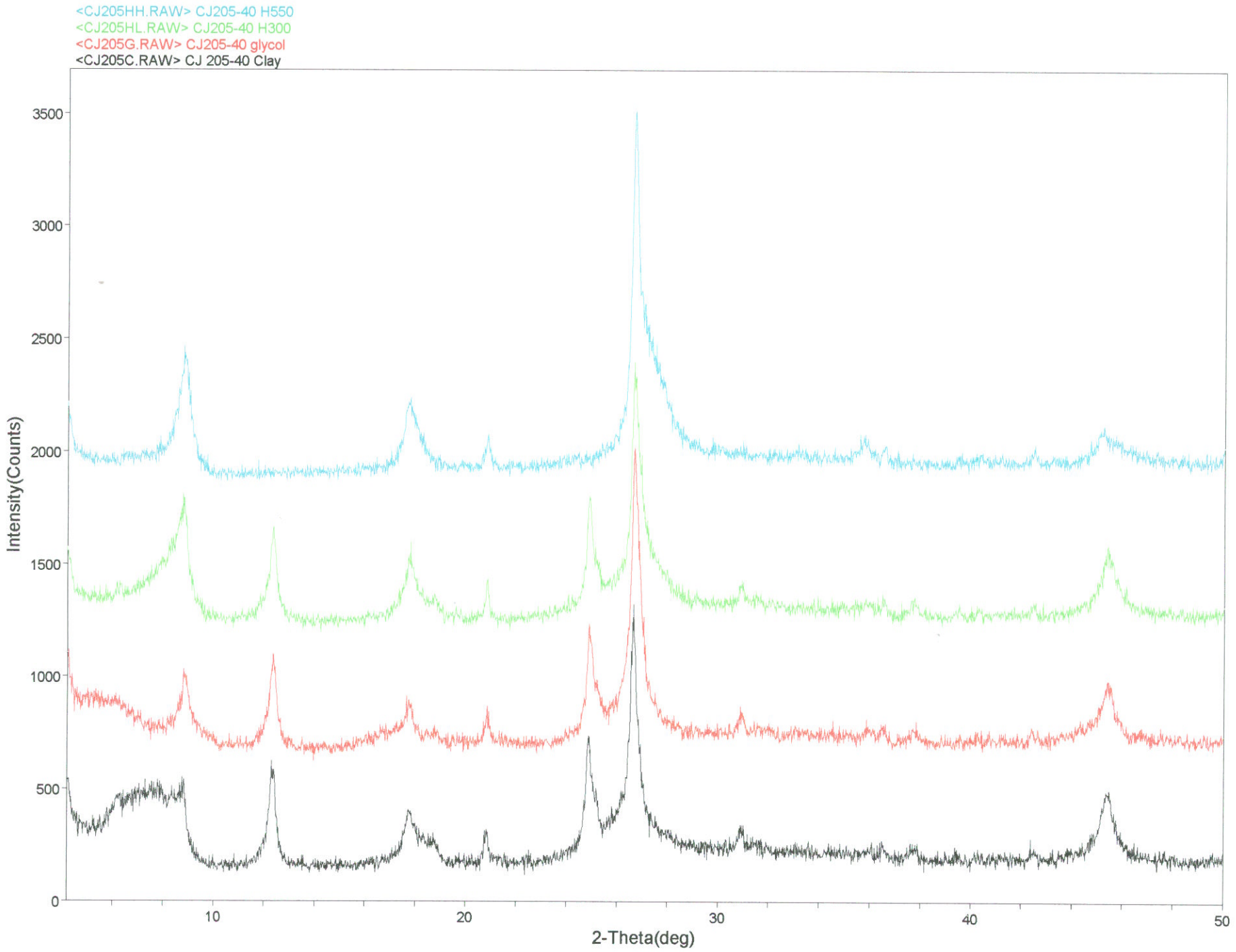

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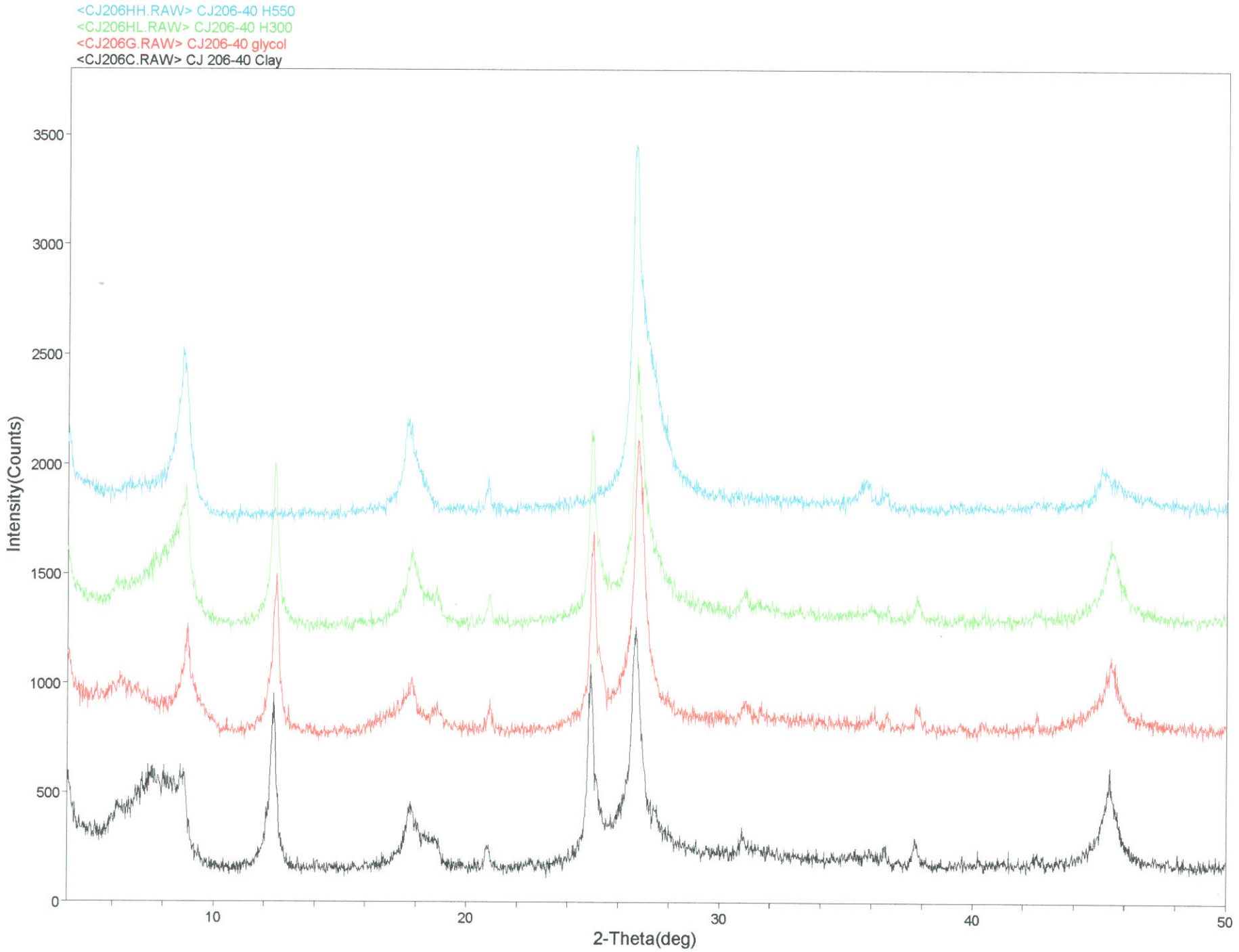

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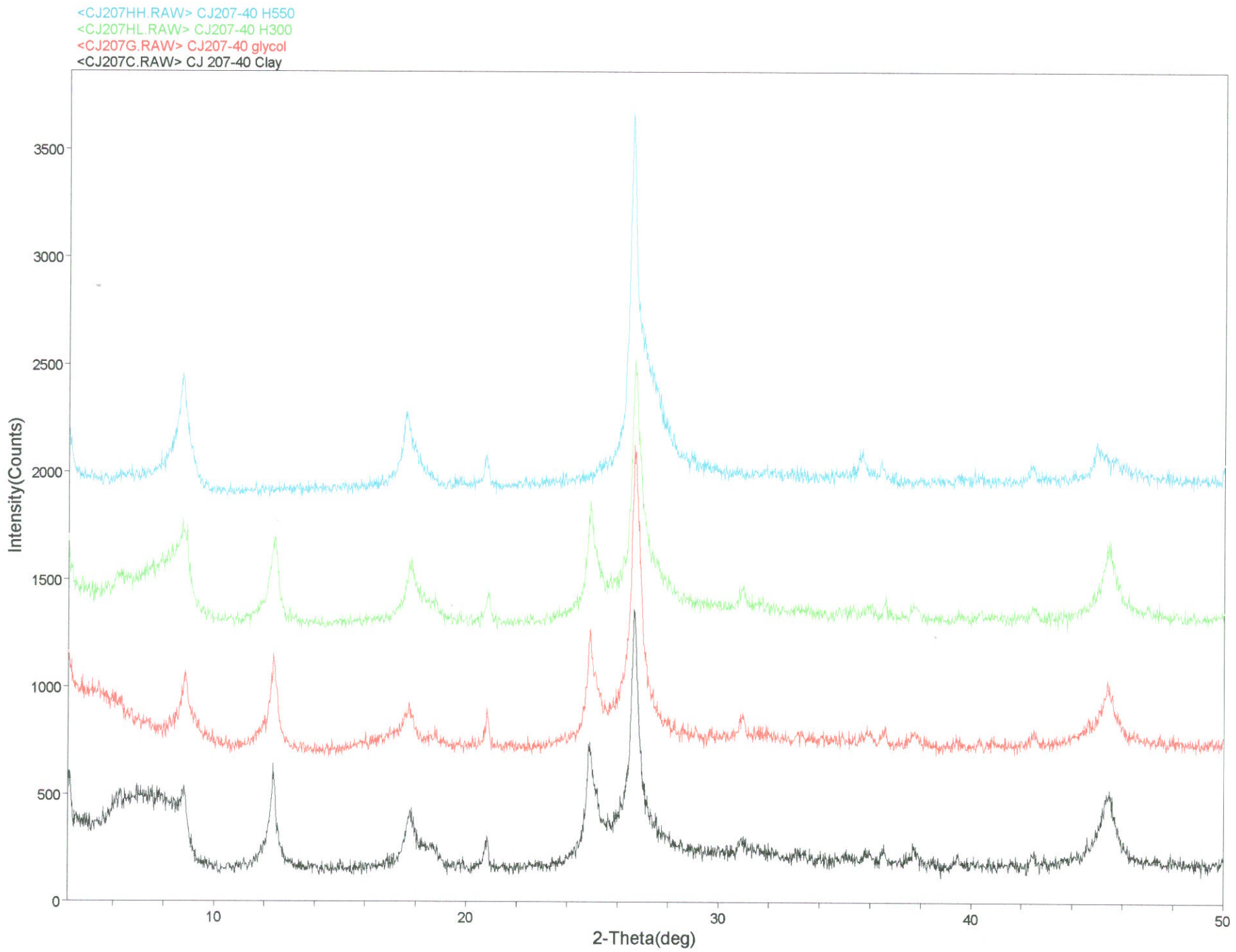

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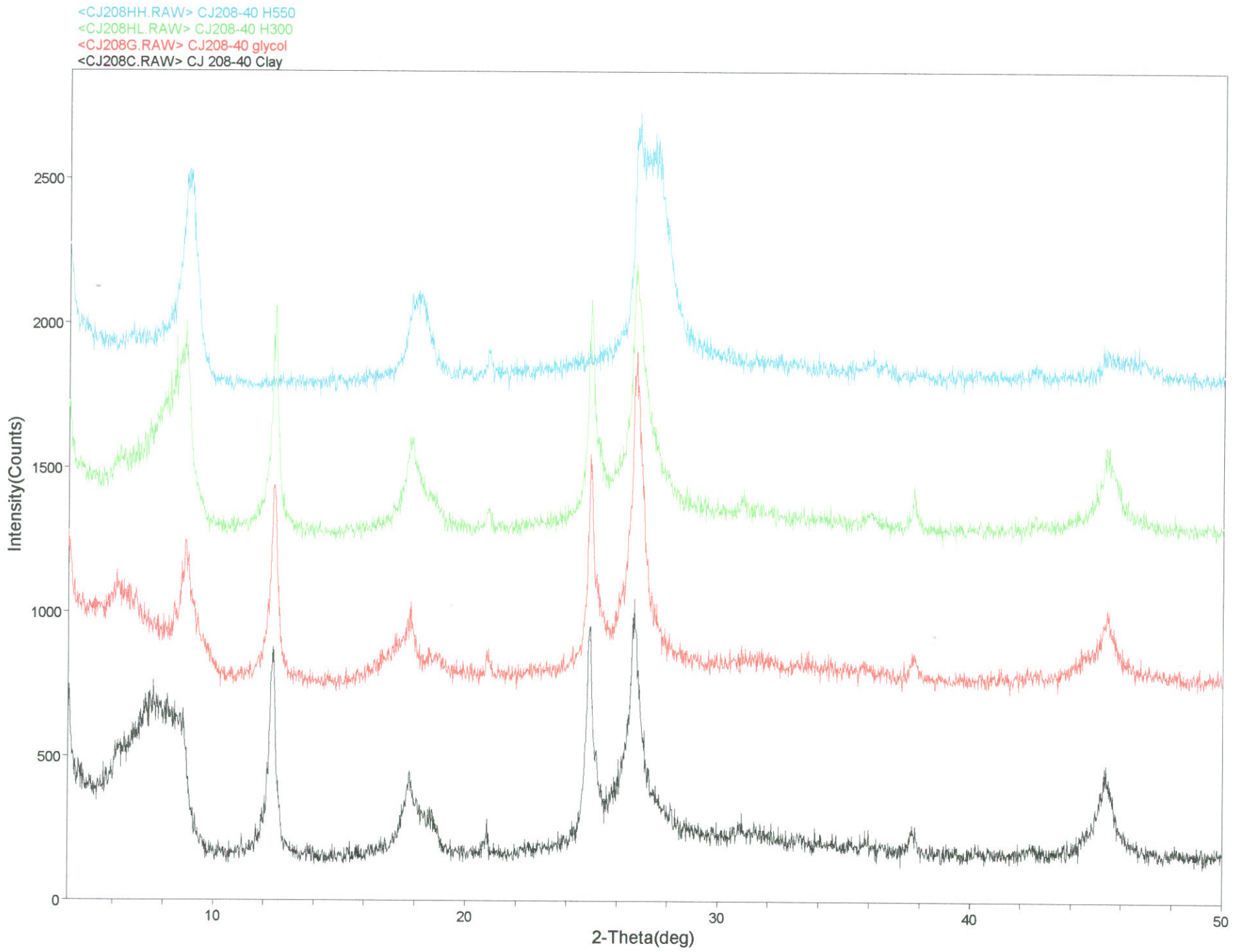

Mesa State College

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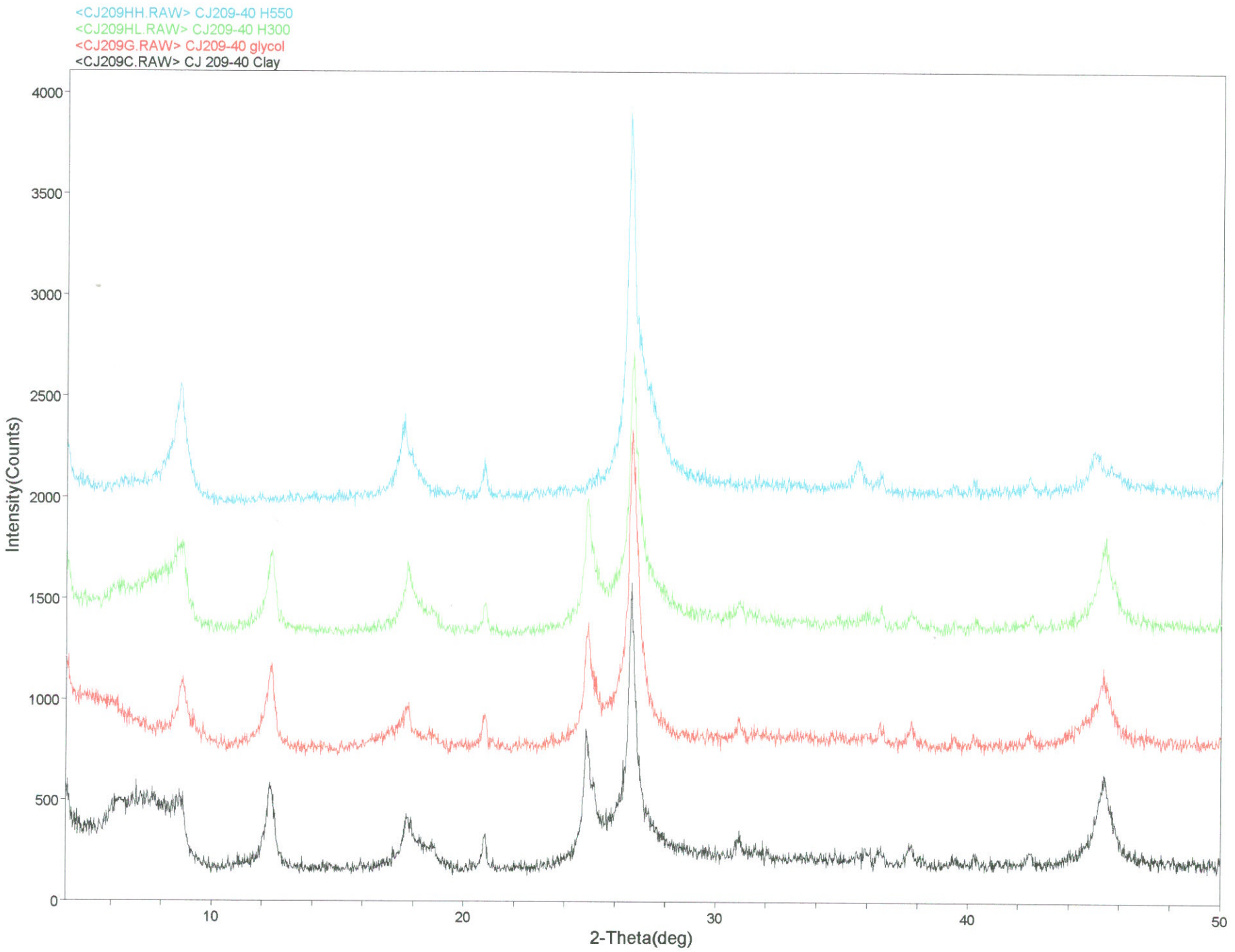

Mesa State College

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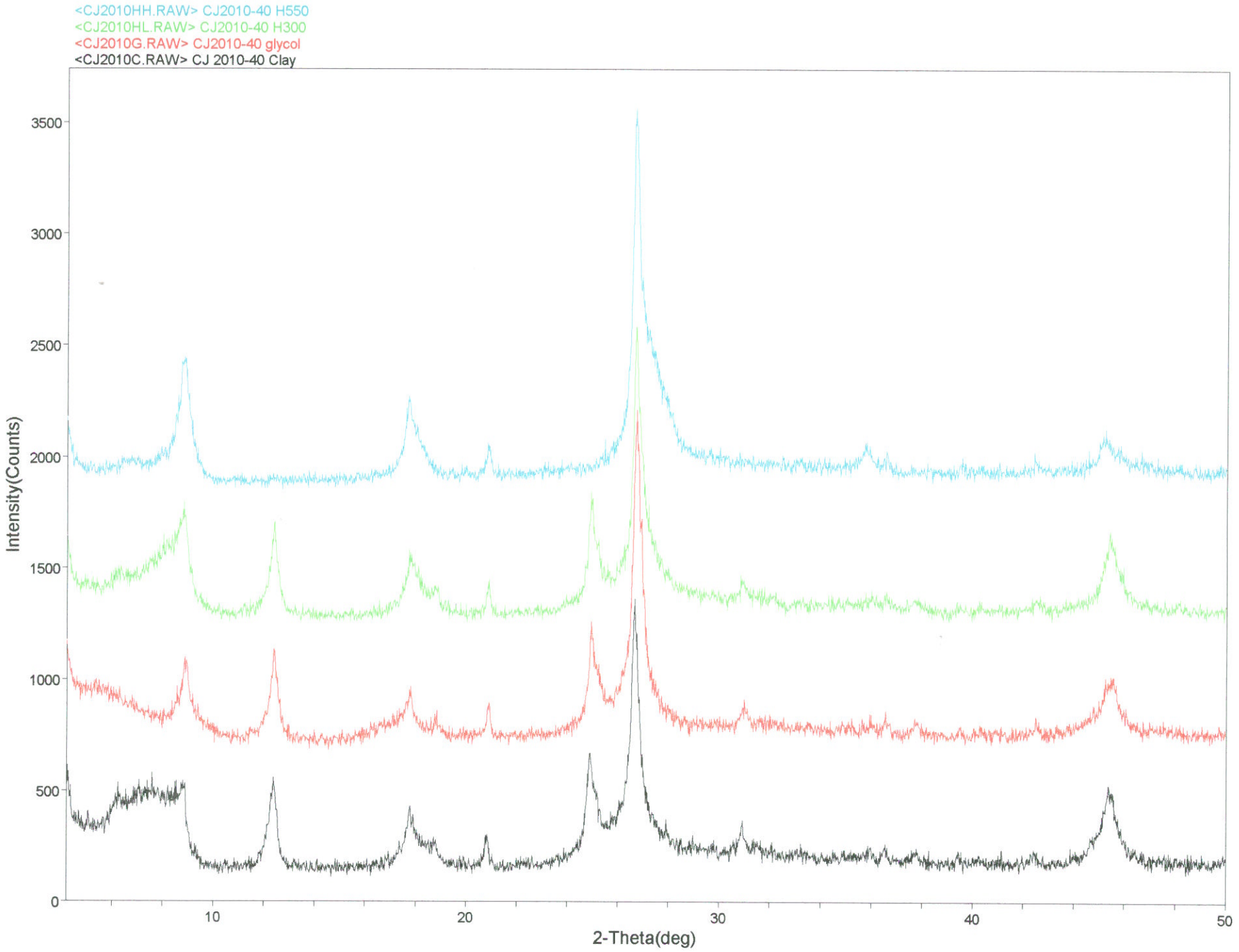


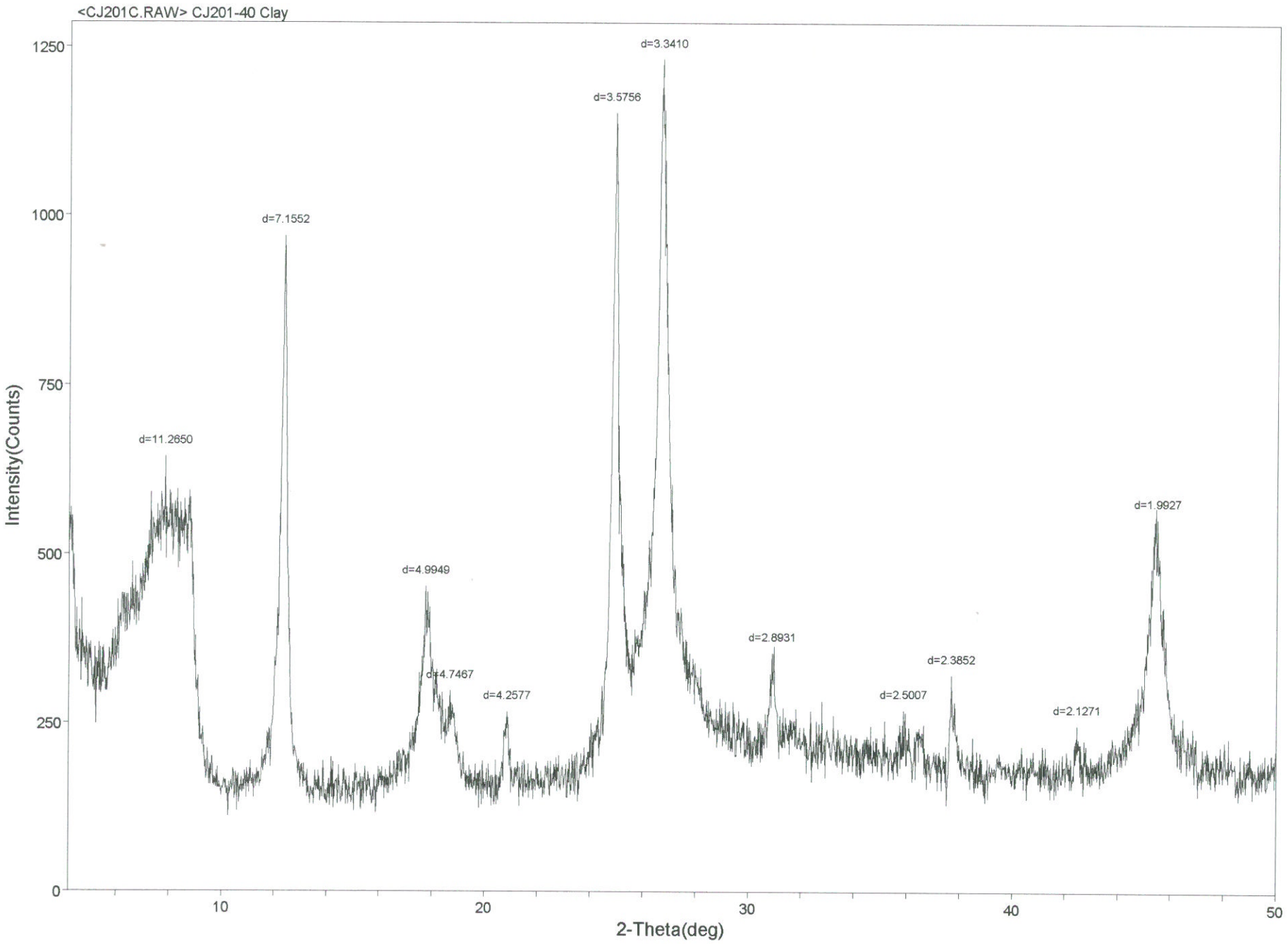
Mesa State College

<c:\hood\doe> Sunday, Jan 29, 2006 @03:19p

Appendix 6.

X-ray diffraction patterns of clay minerals in CJ sample set

Patterns are arranged in the sequence: untreated, glycol solvated, heated to 300° C and heated to 500° C for each sample.



Mesa State College

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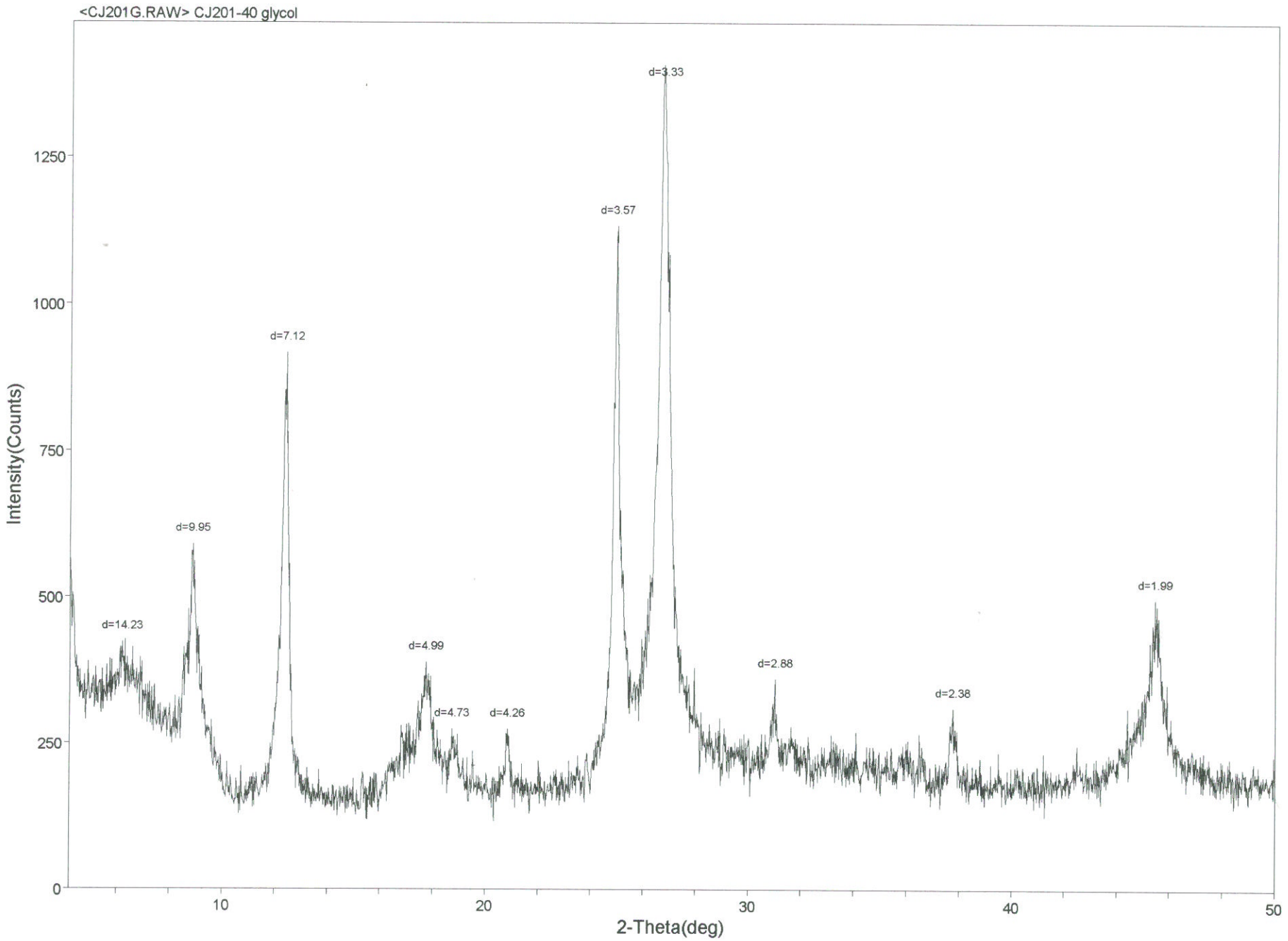

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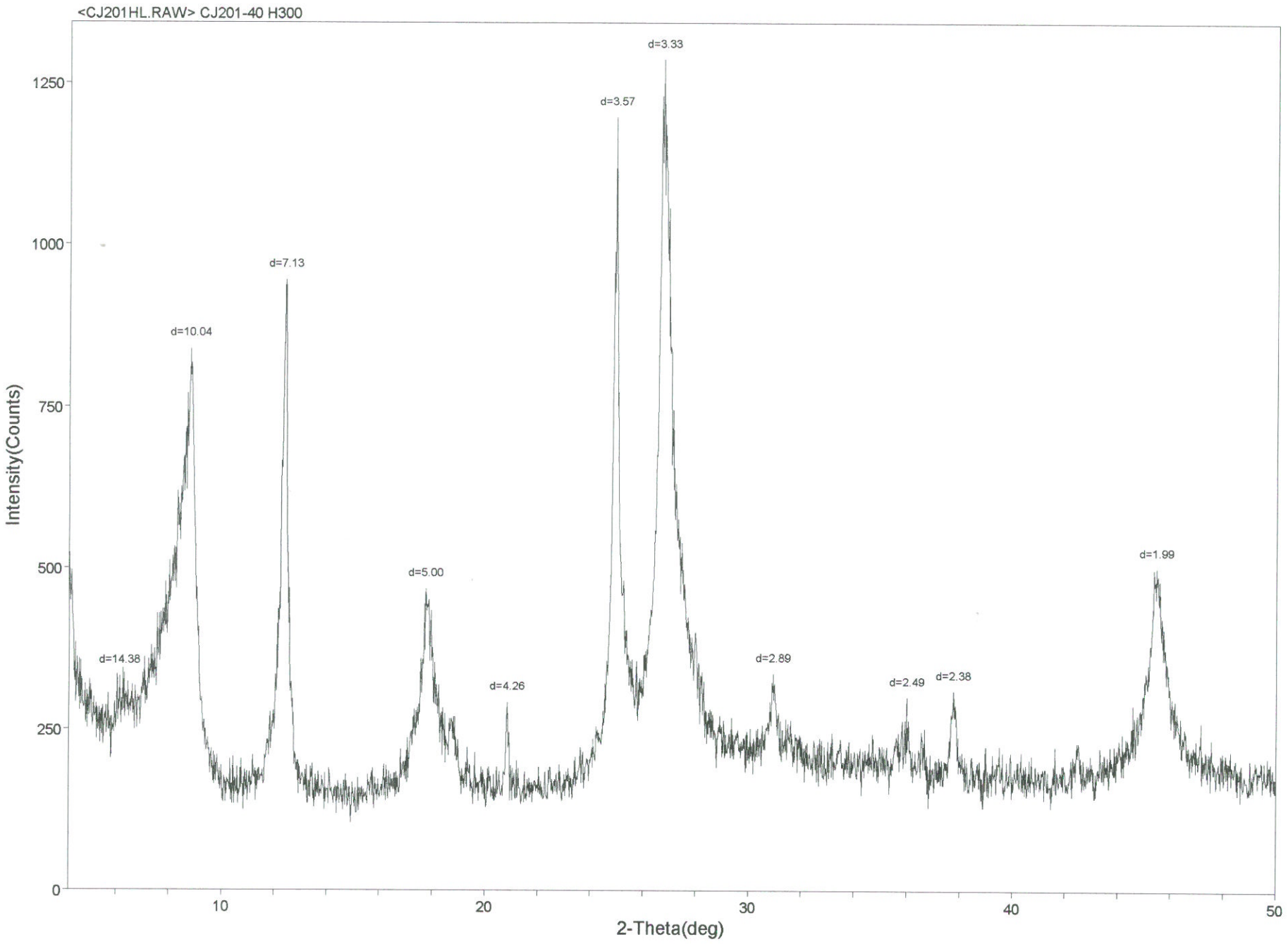

Mesa State College

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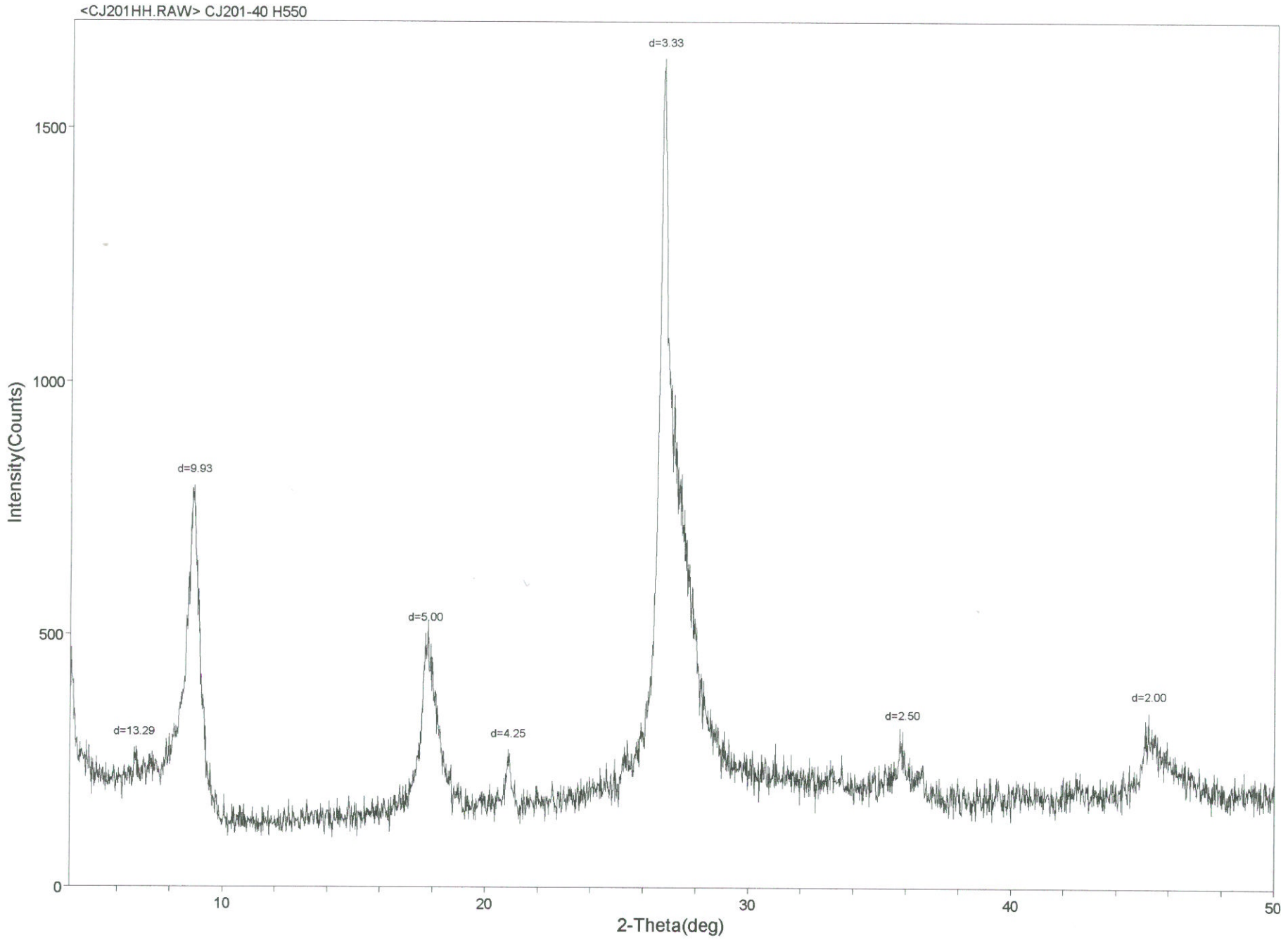

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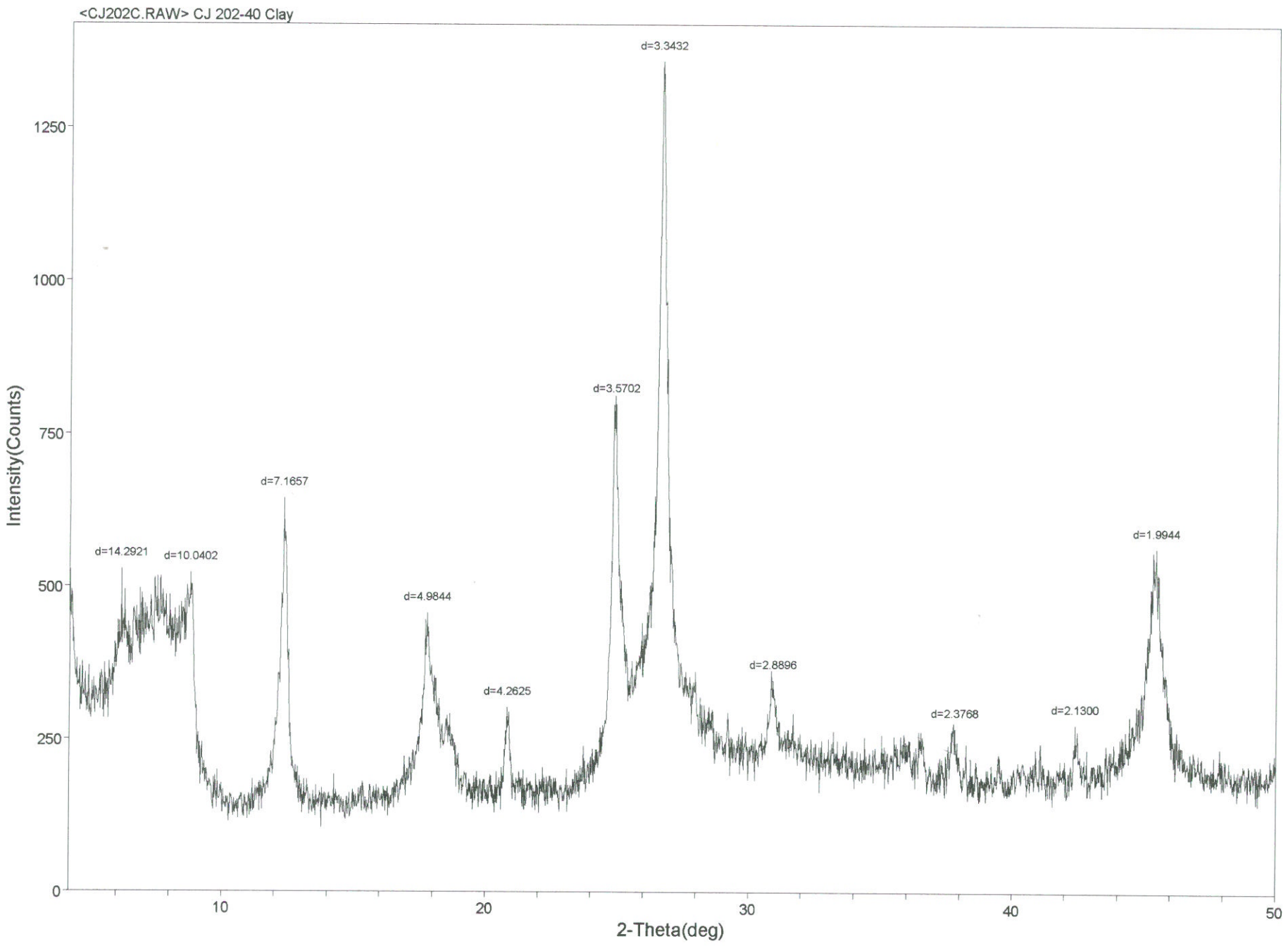

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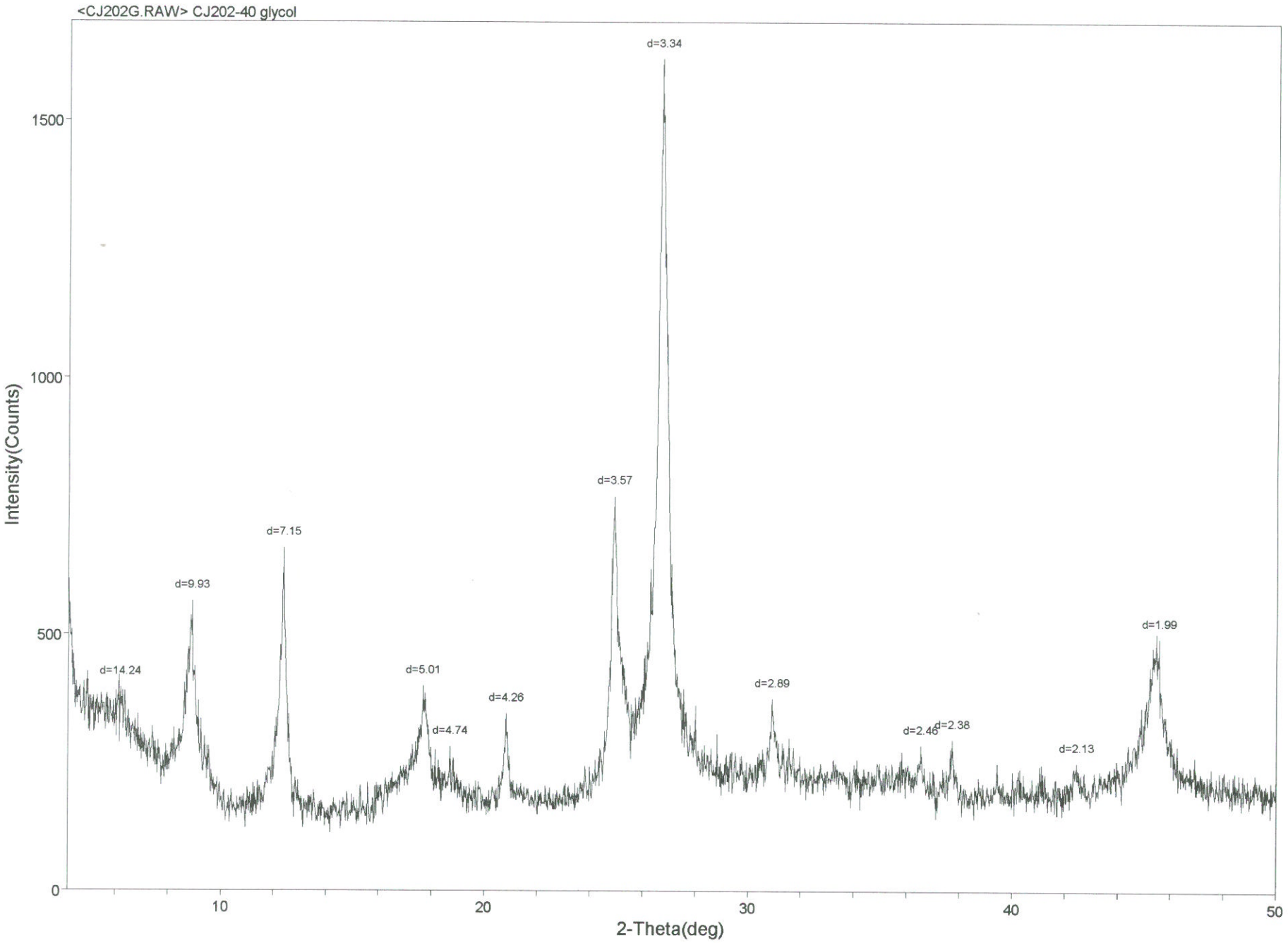

Mesa State College

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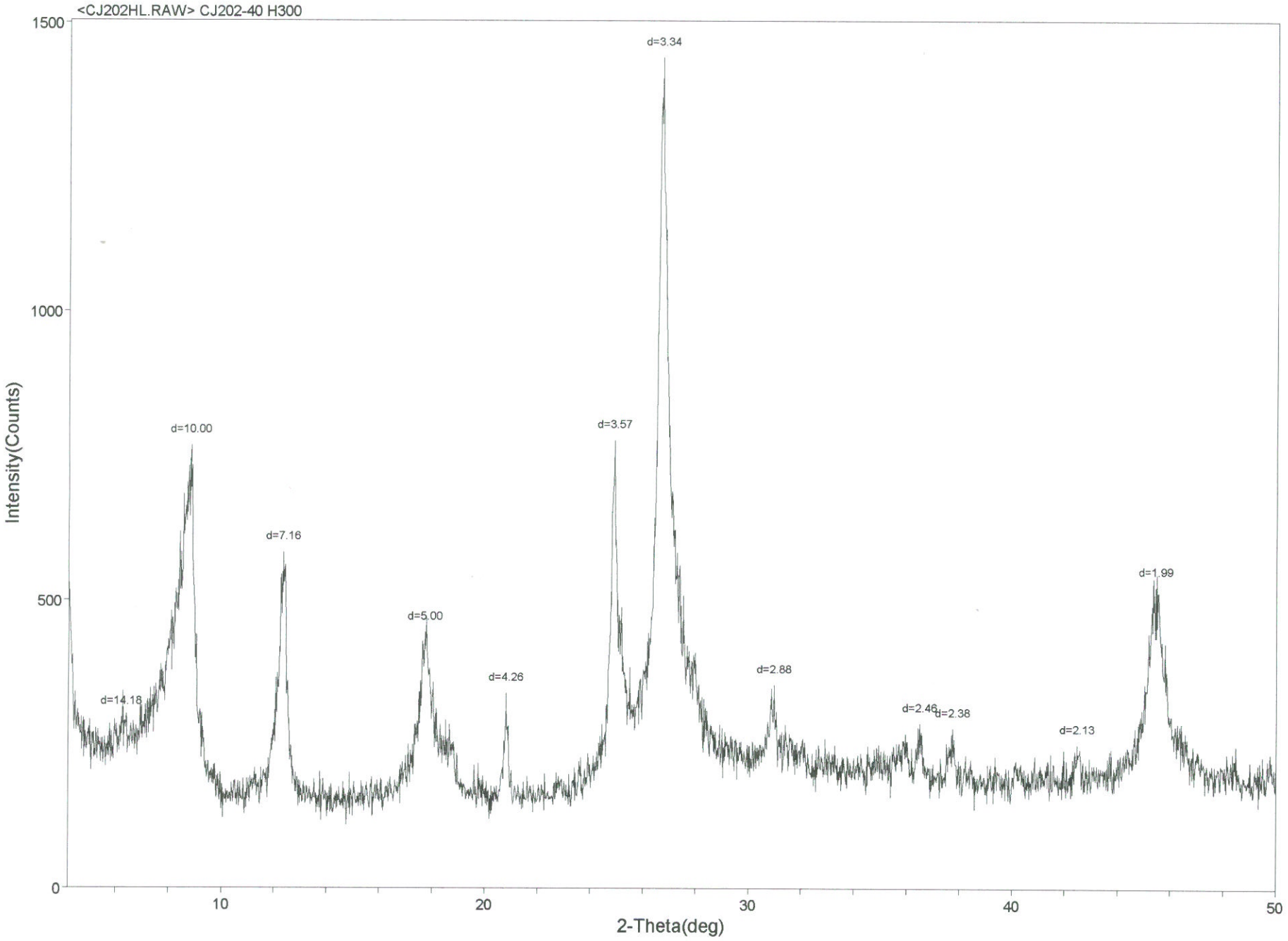

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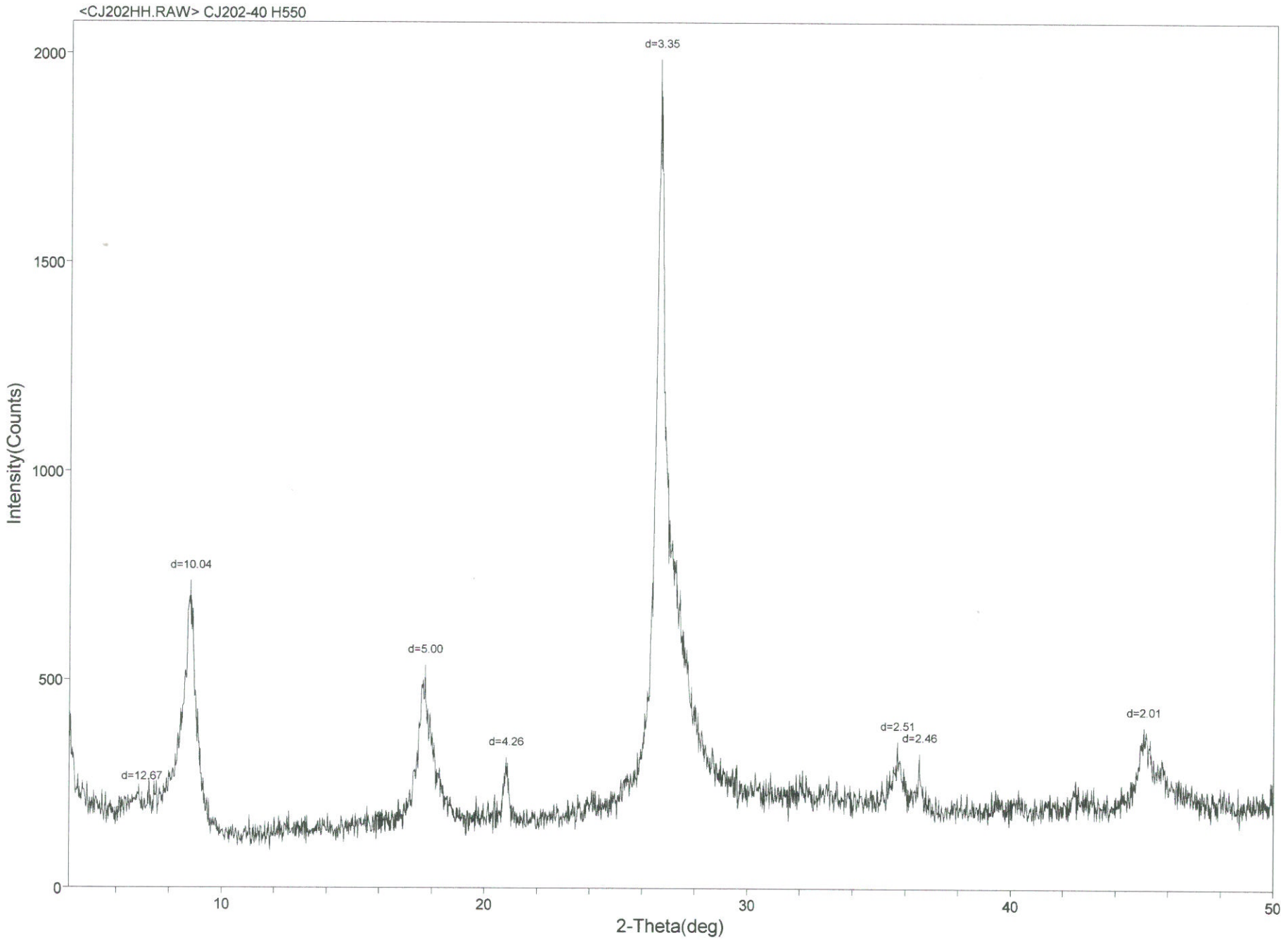

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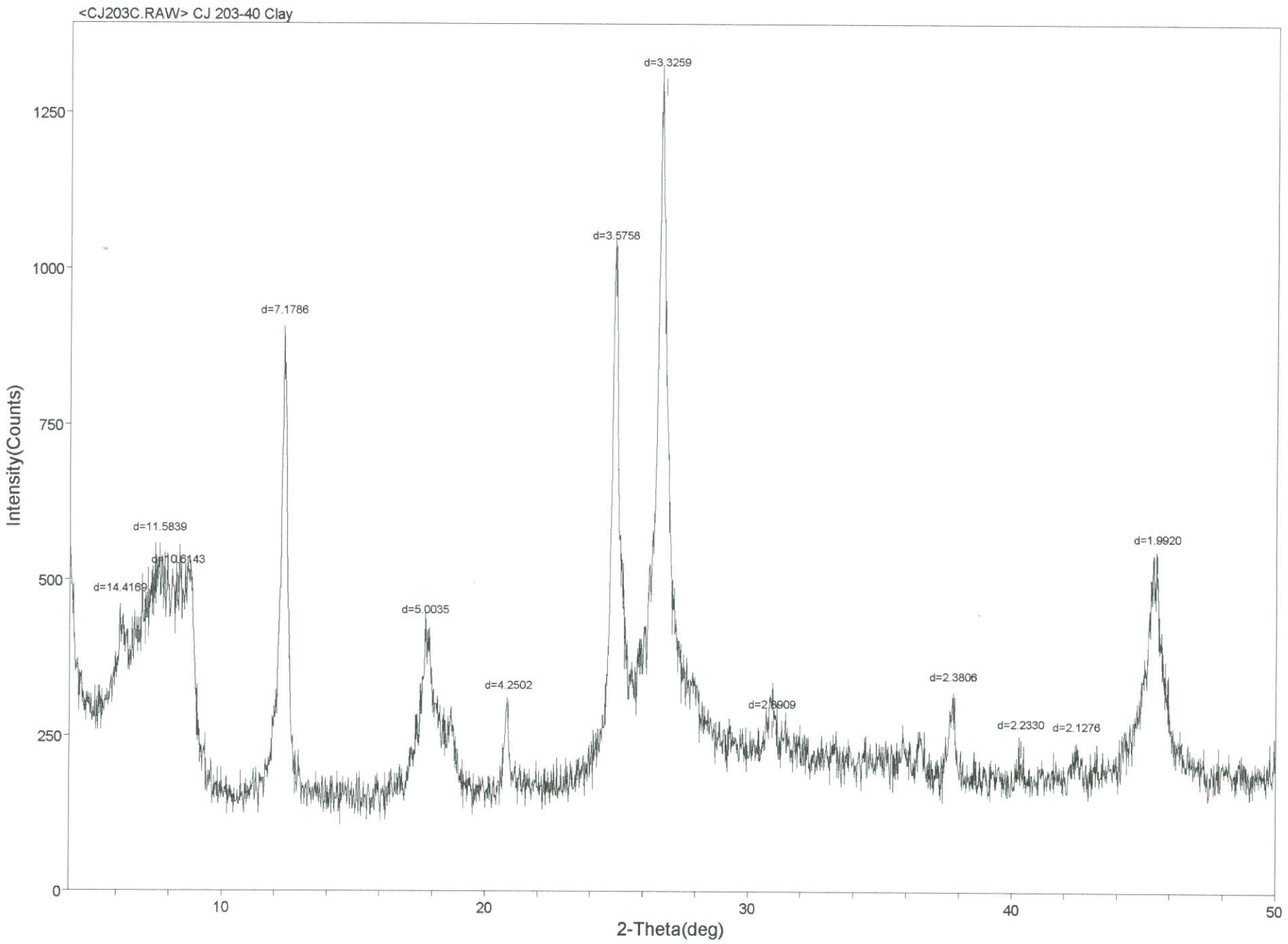

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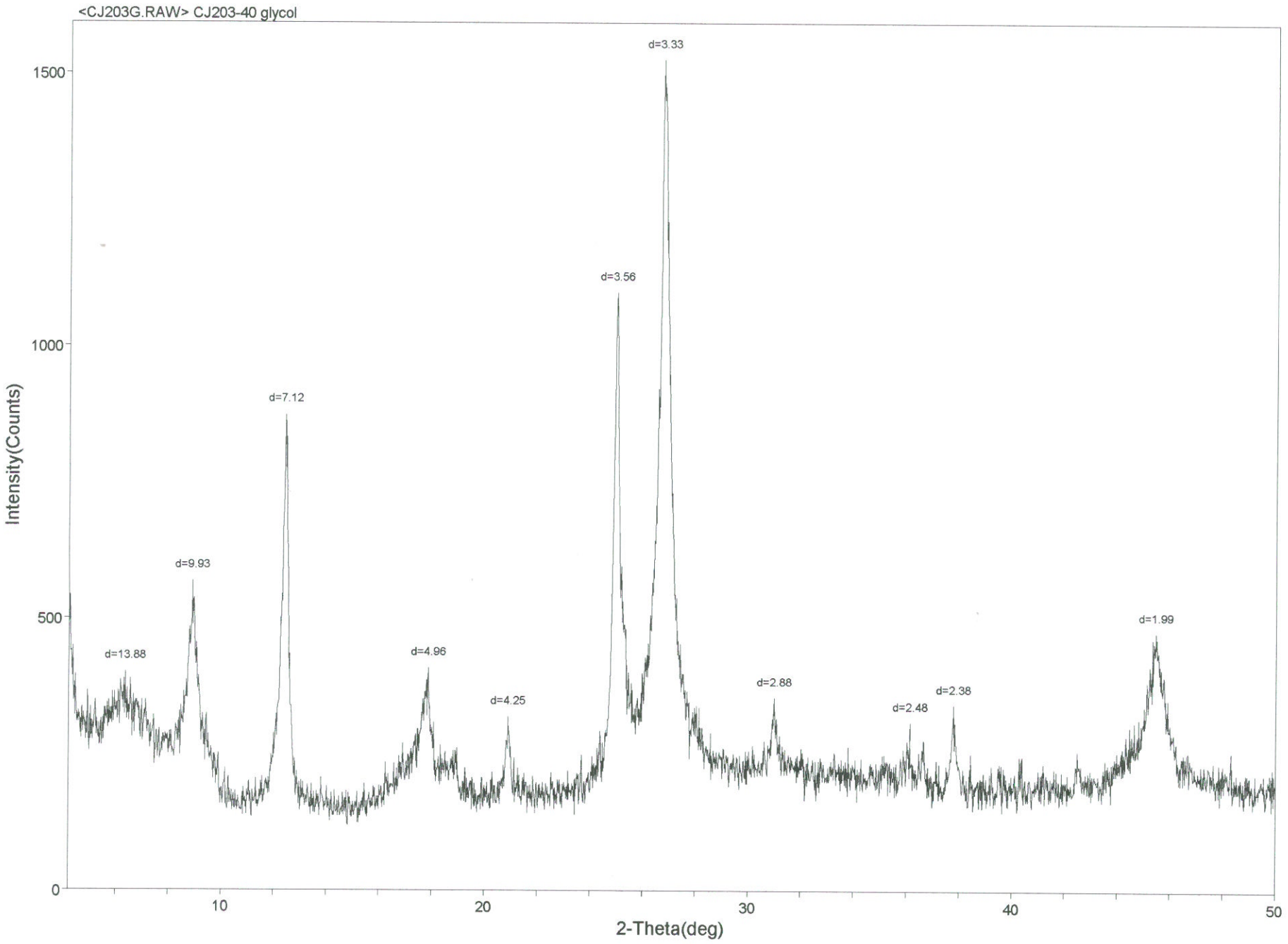

Mesa State College

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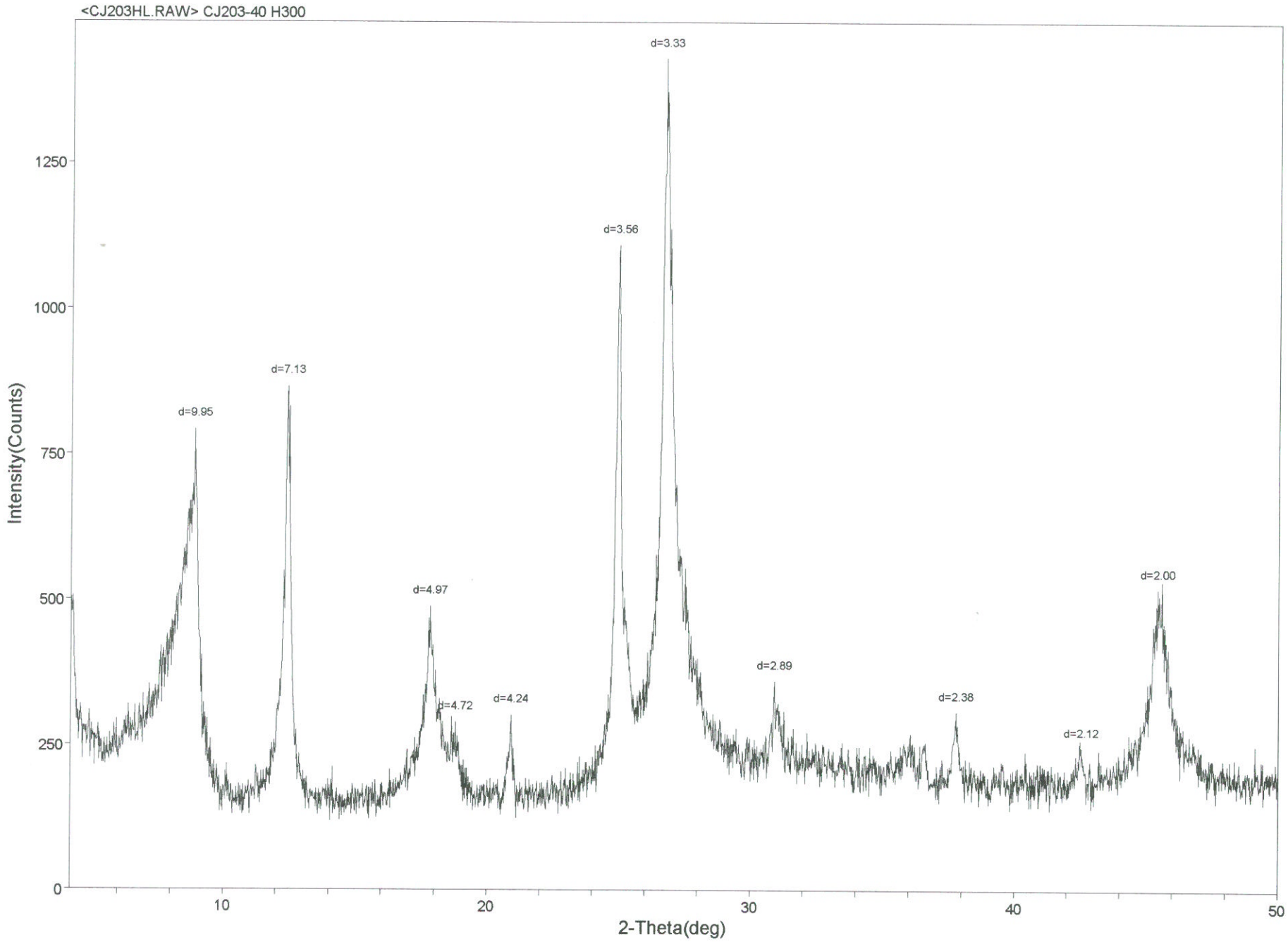

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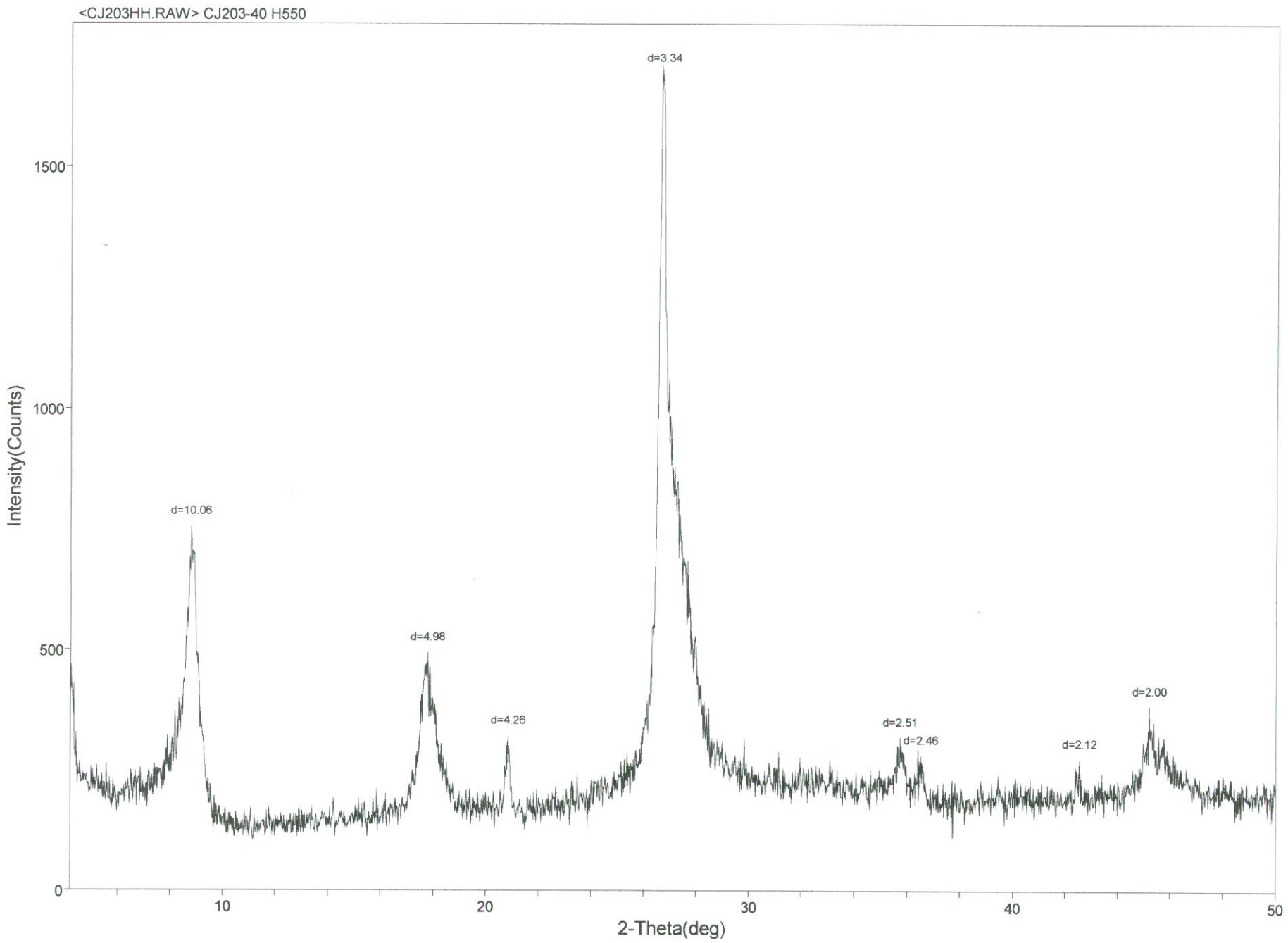

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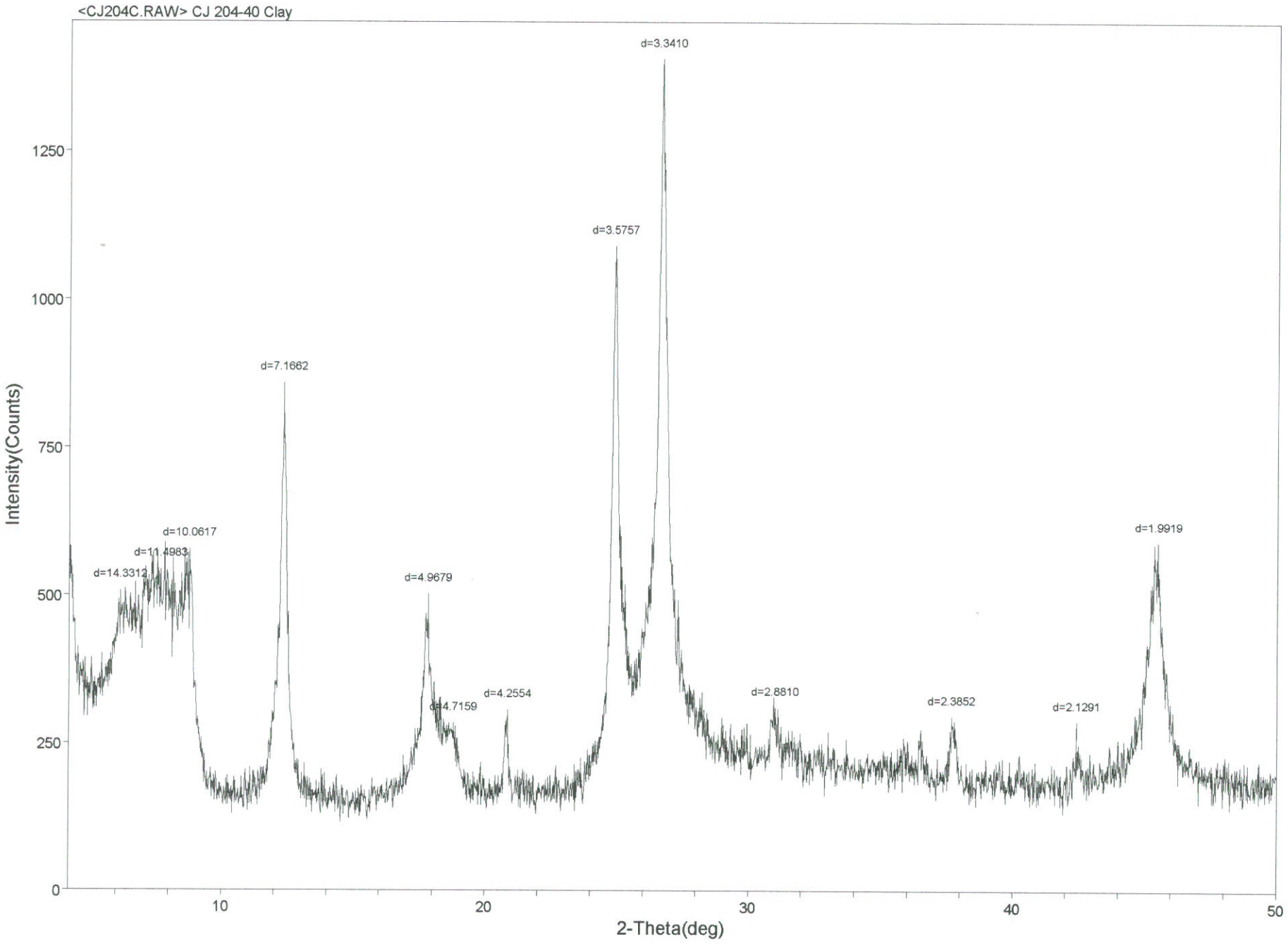

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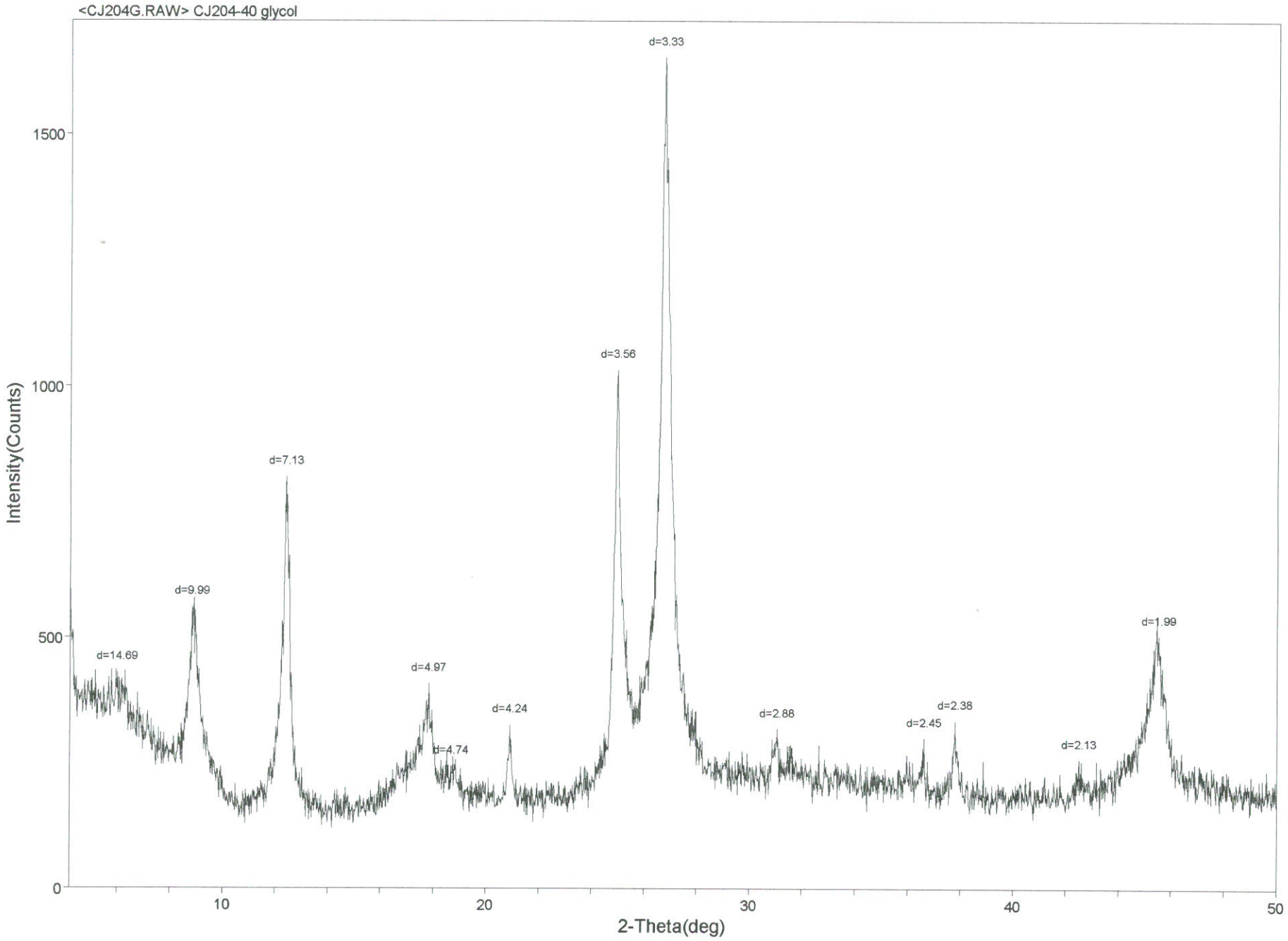

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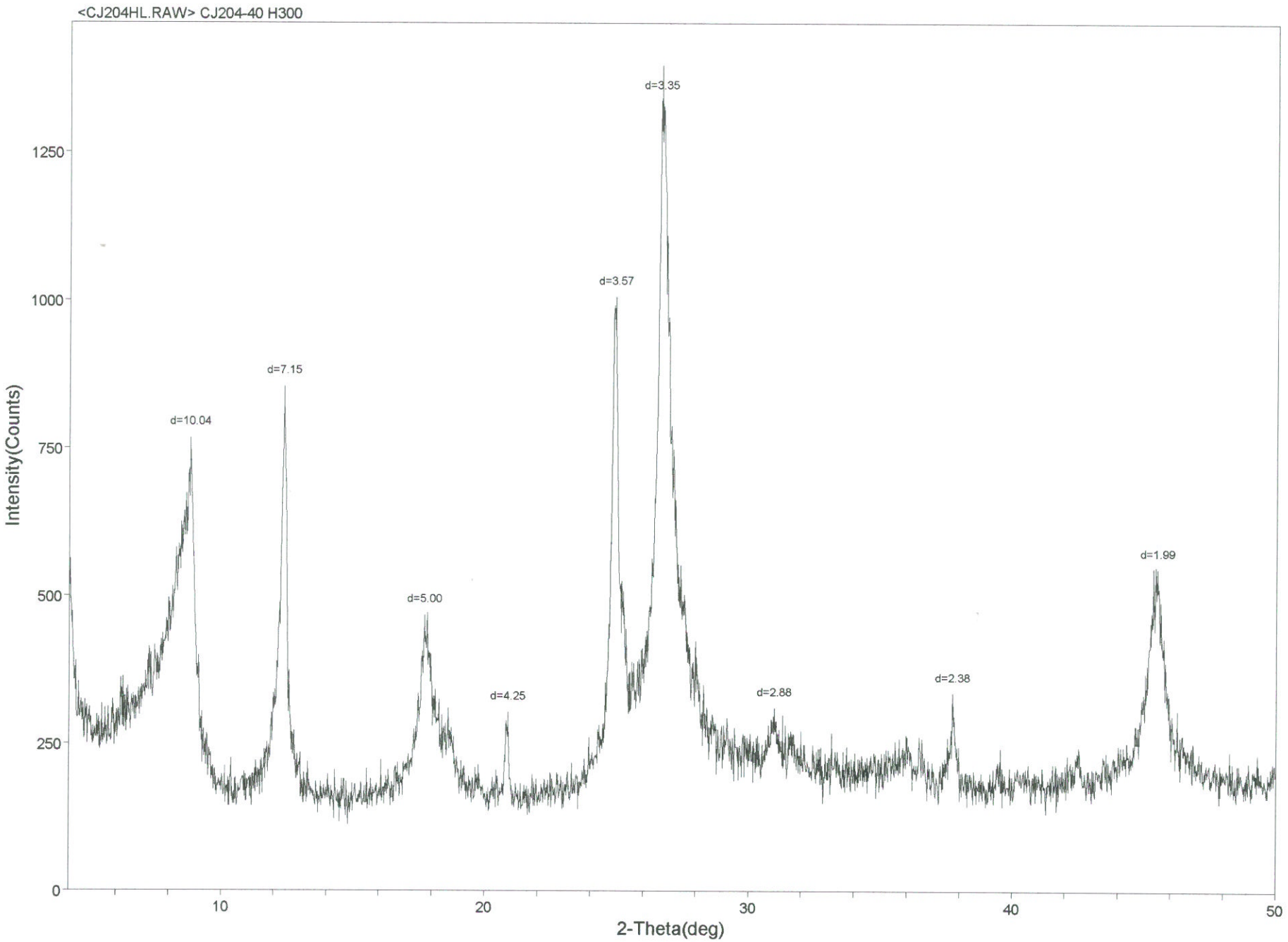

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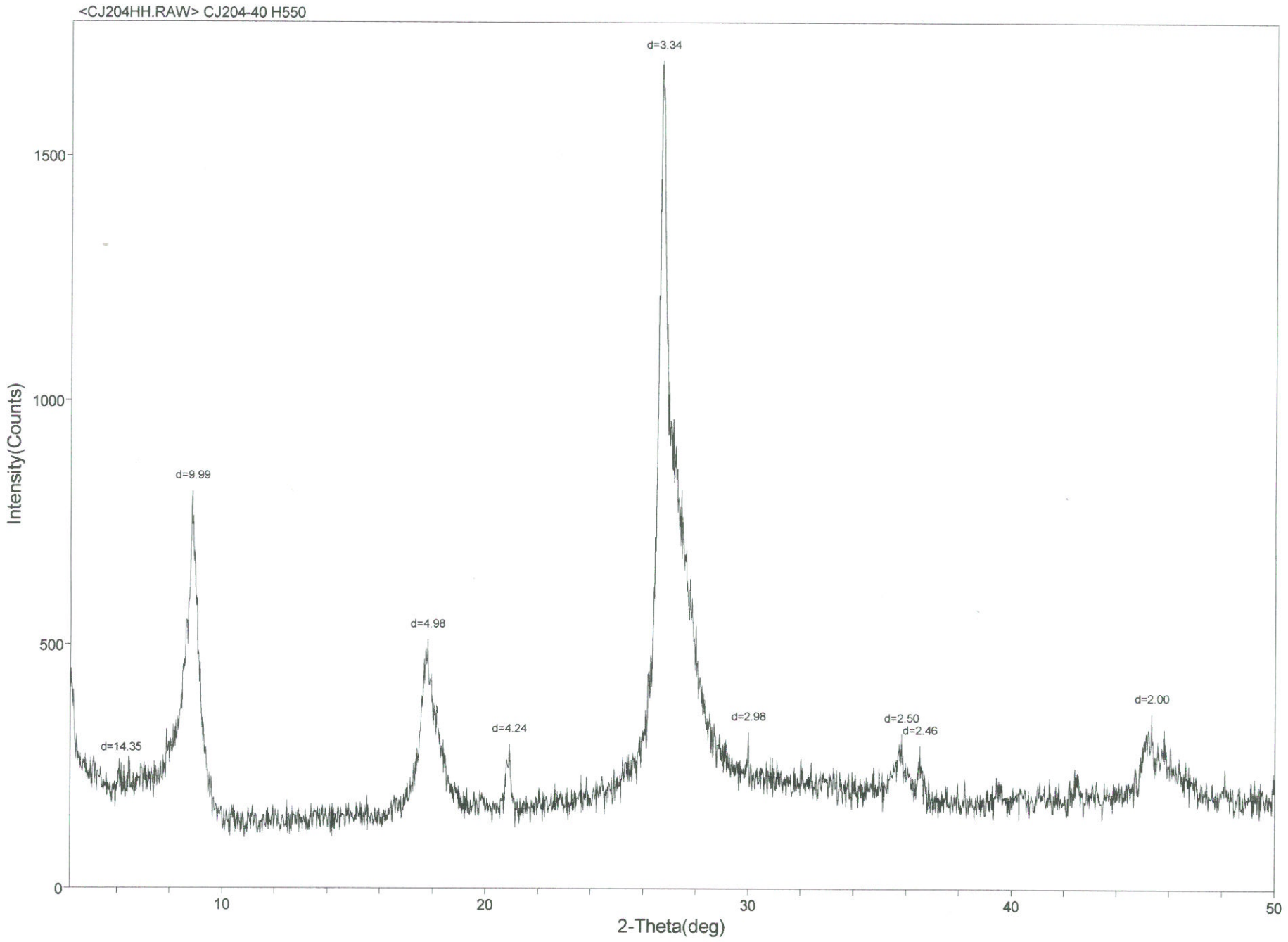

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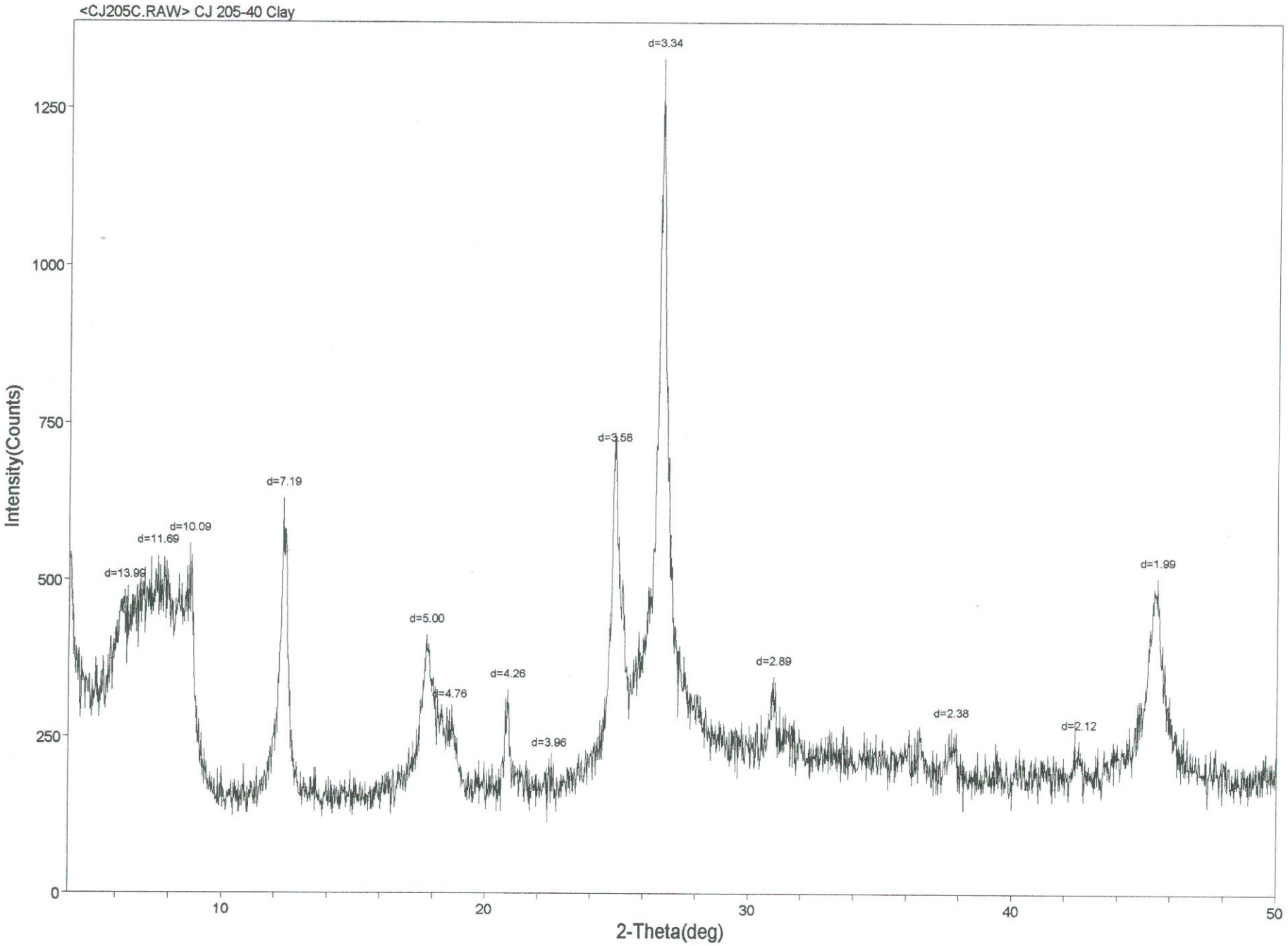

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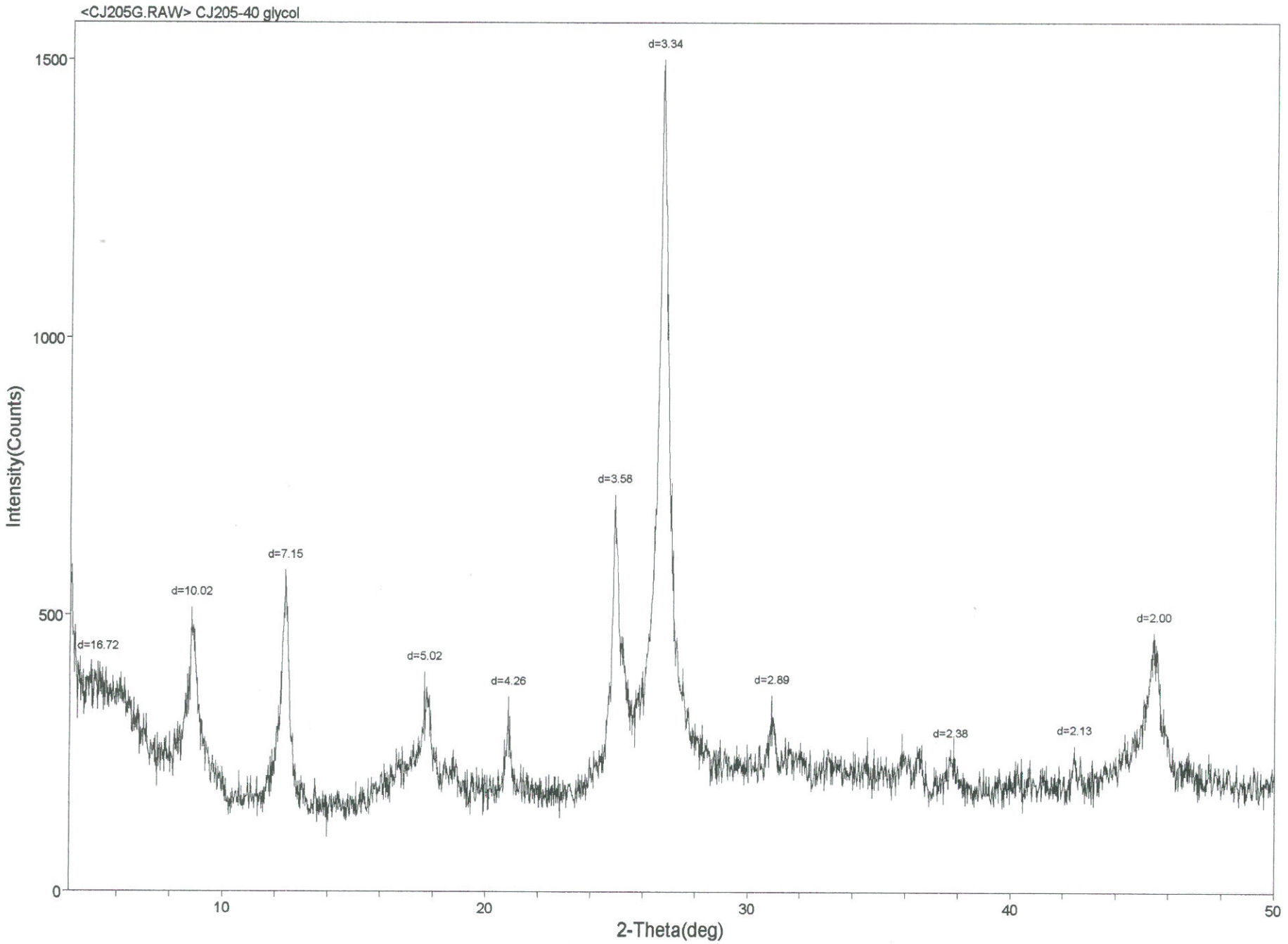

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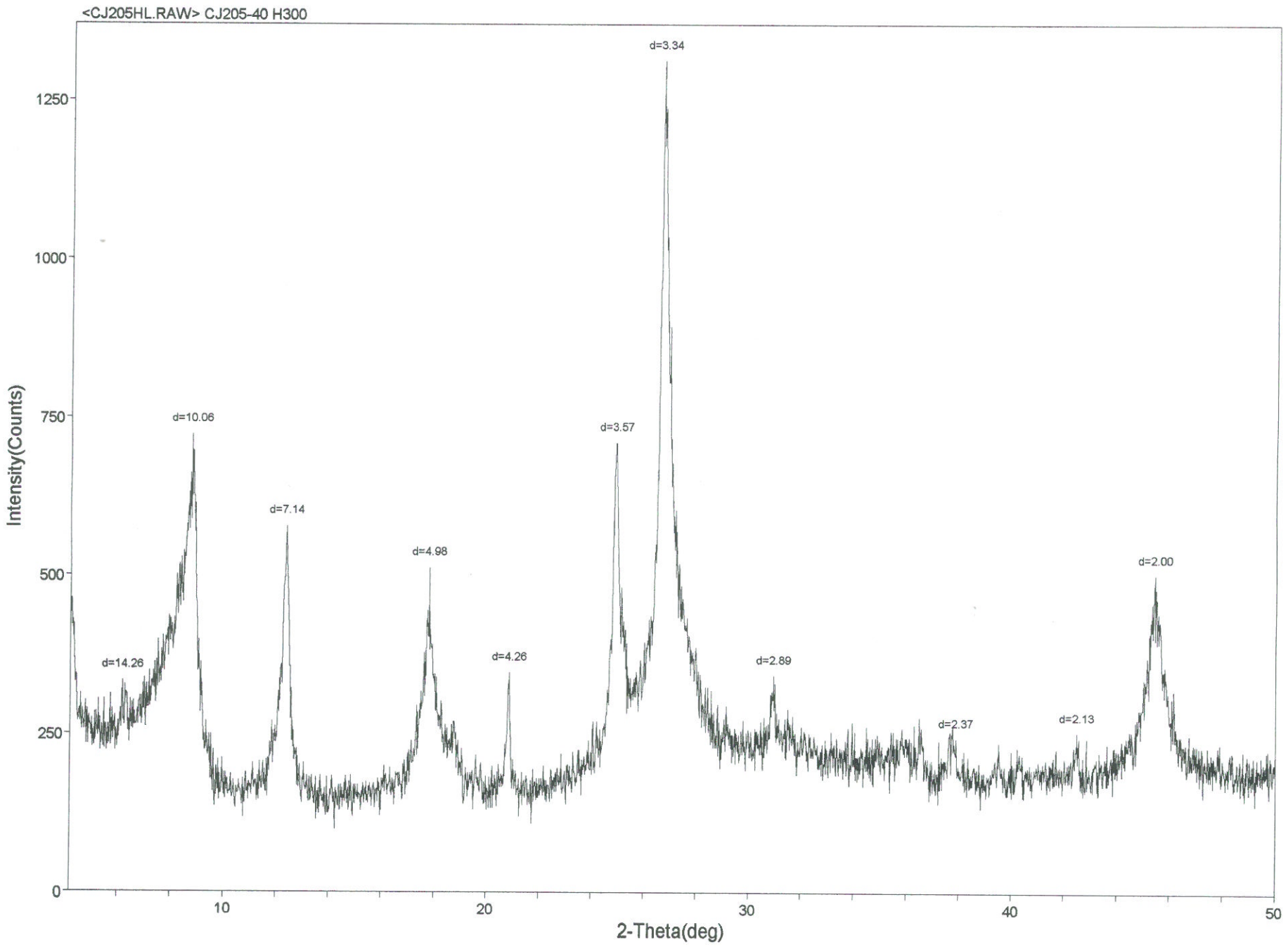

Mesa State College

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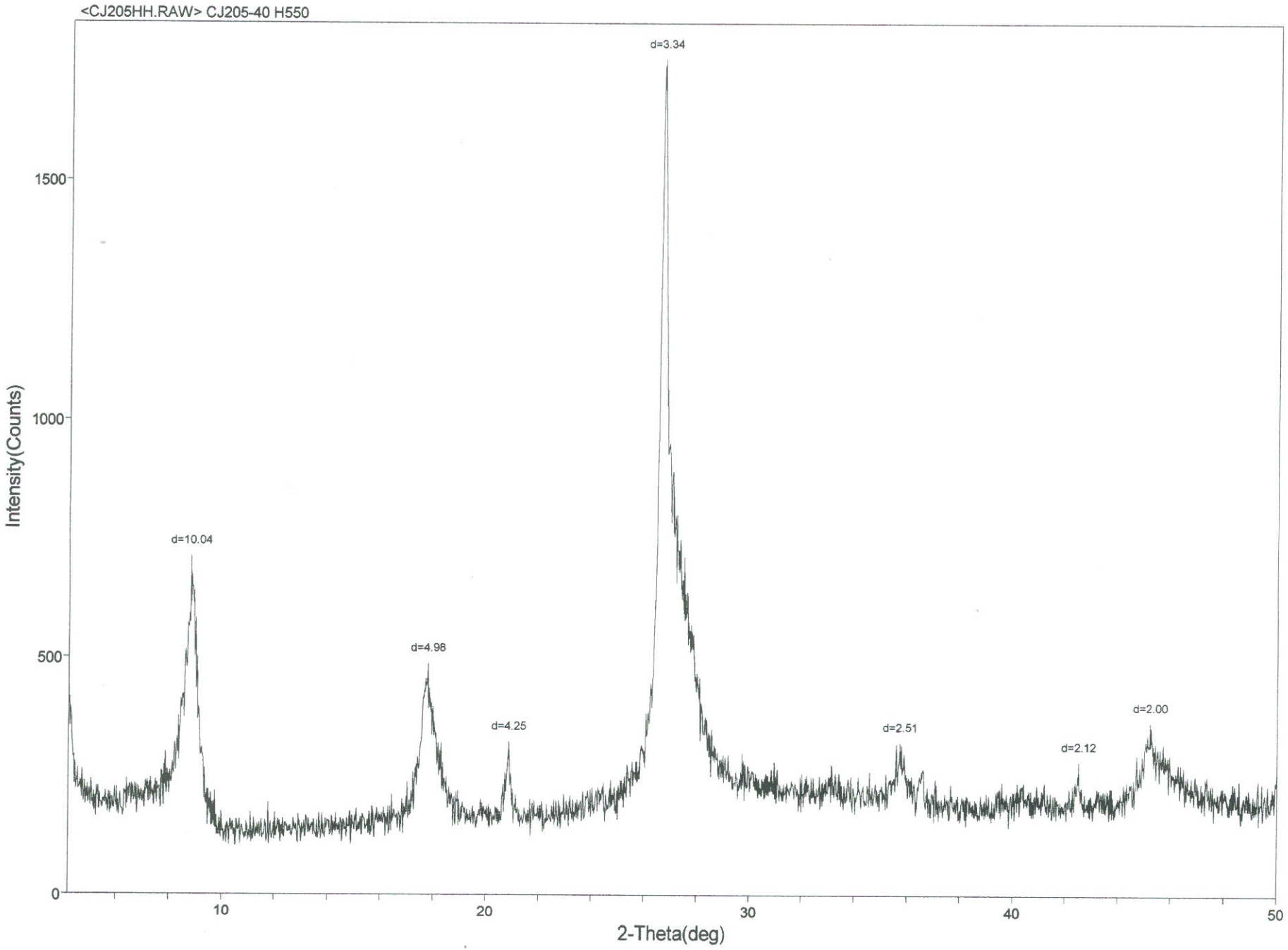

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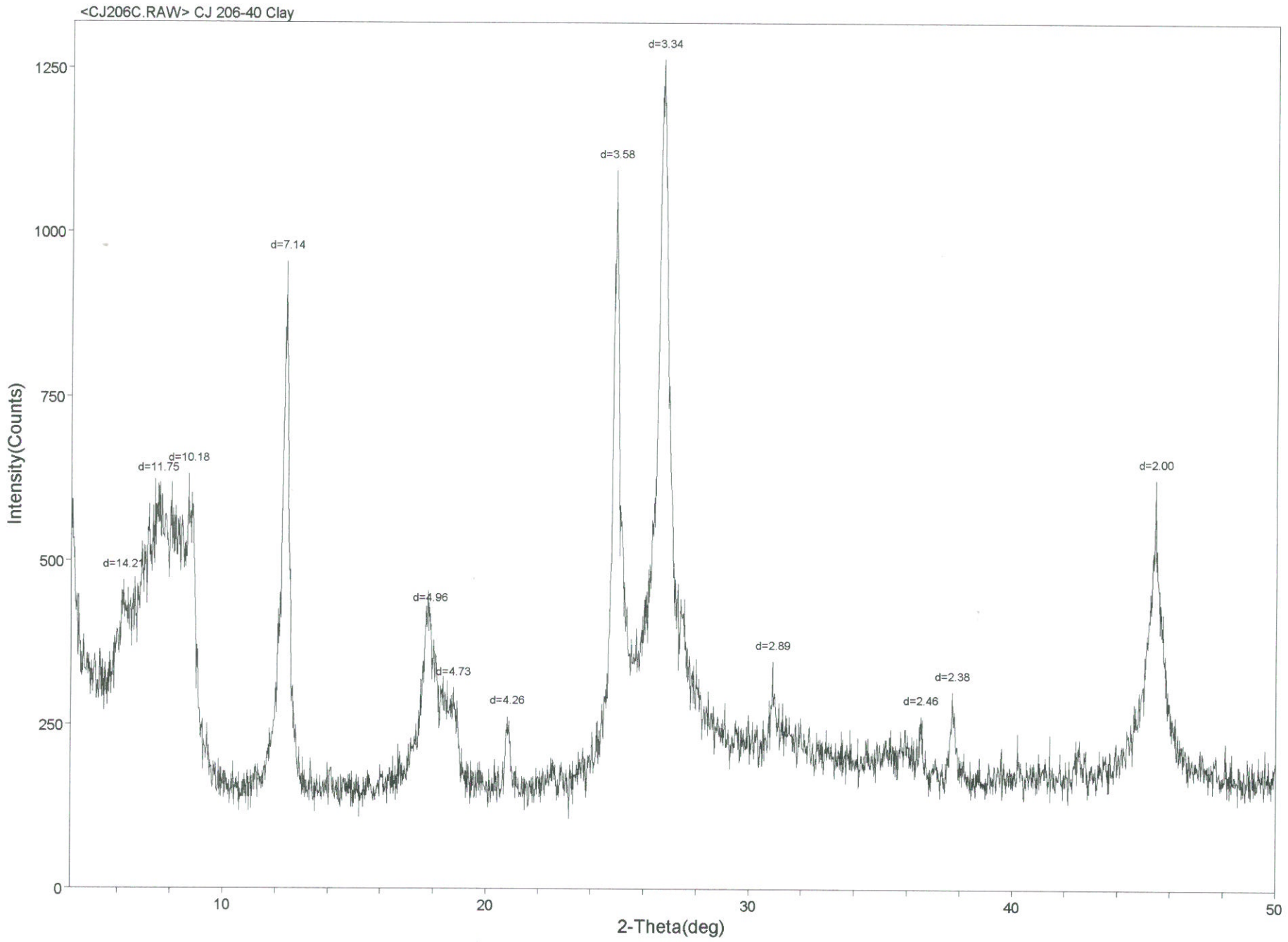

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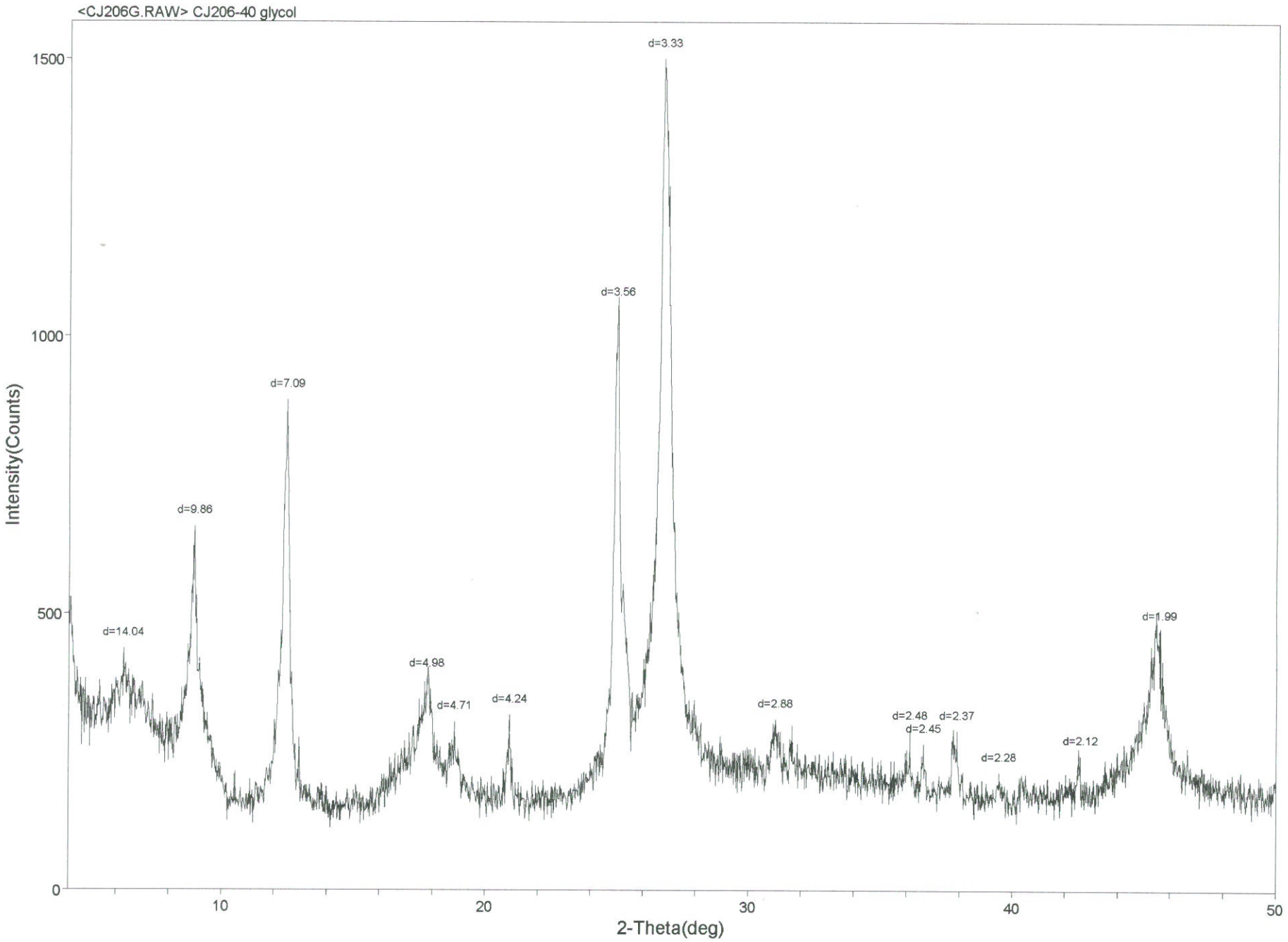

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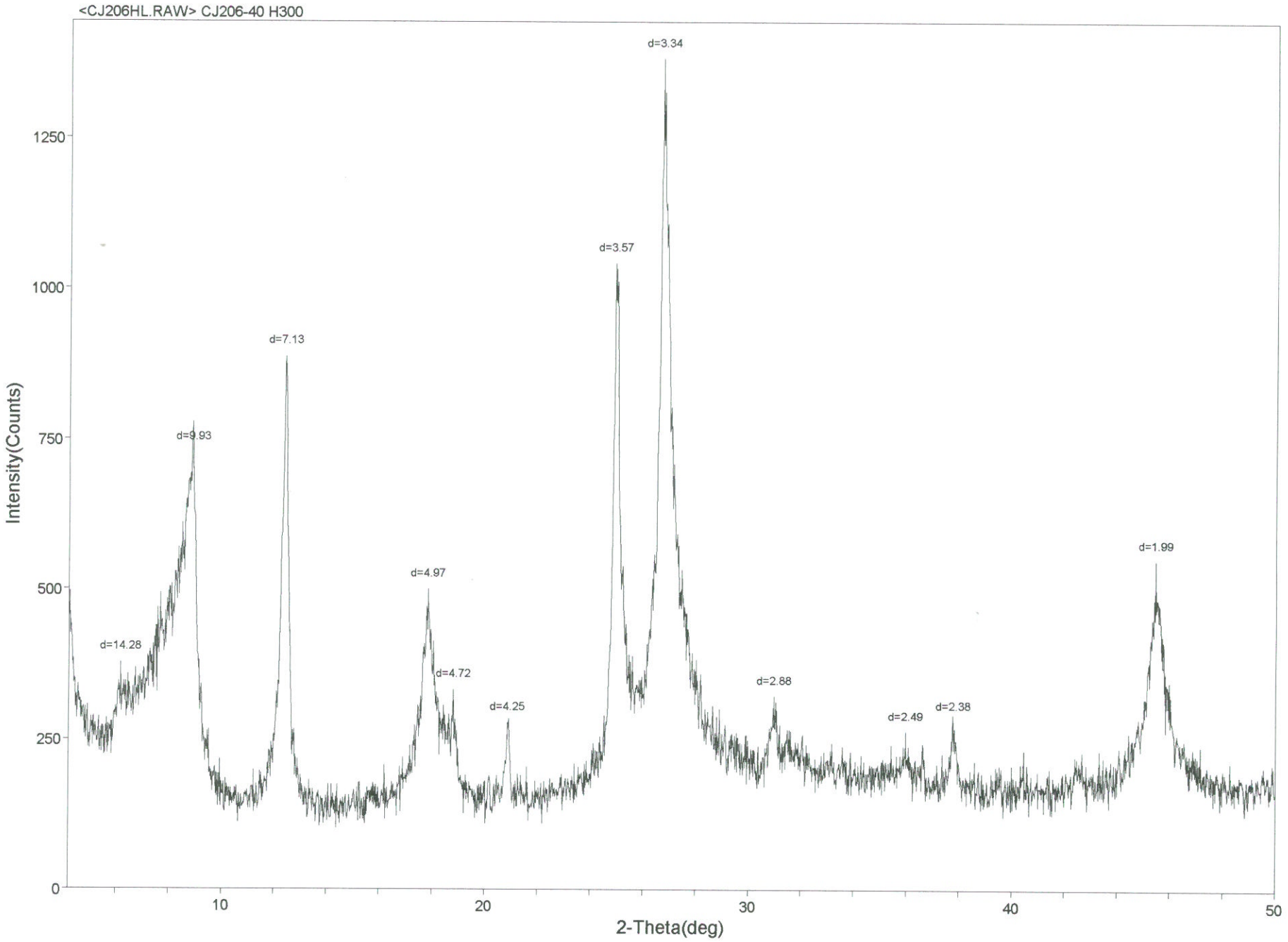

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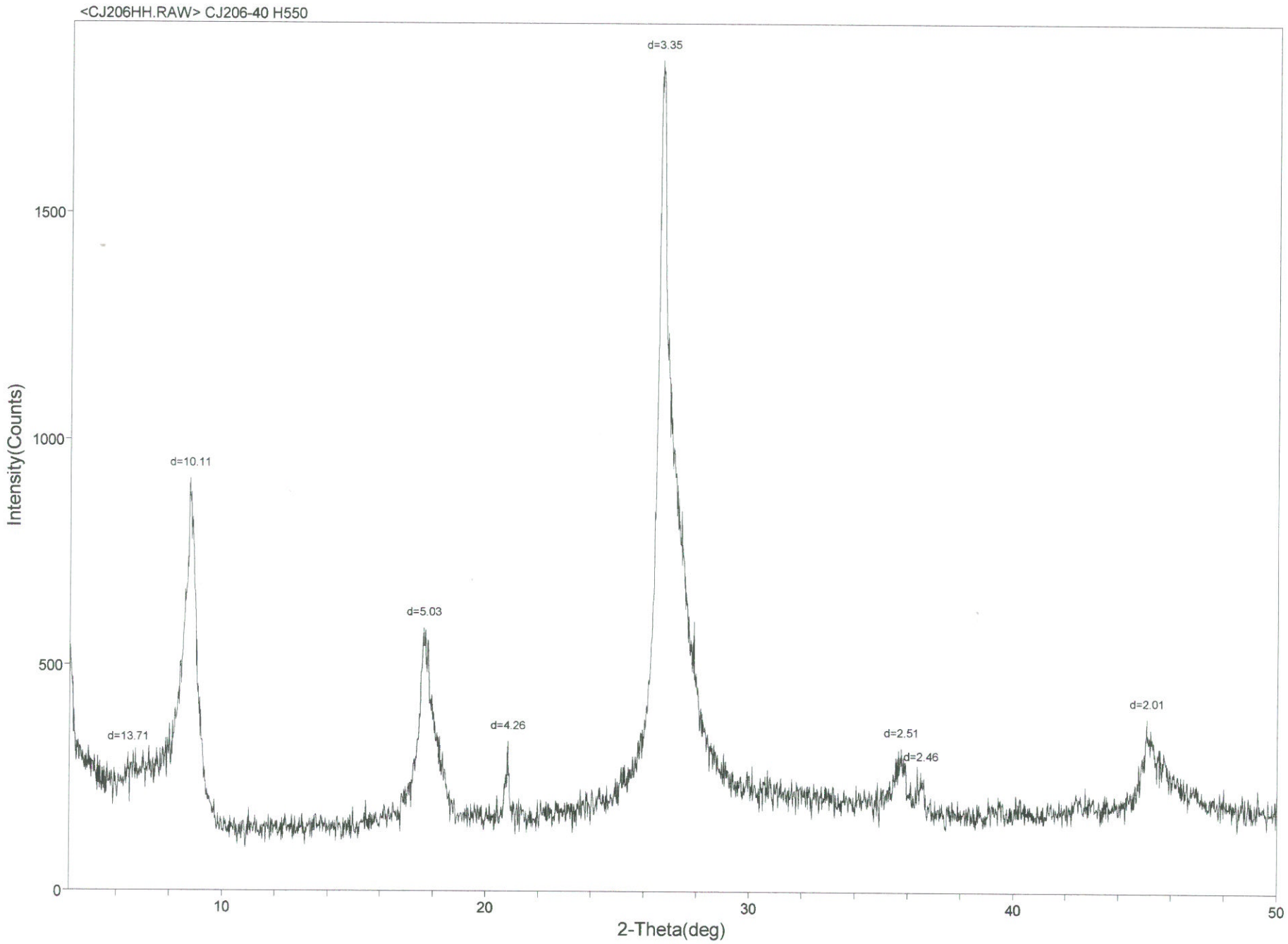

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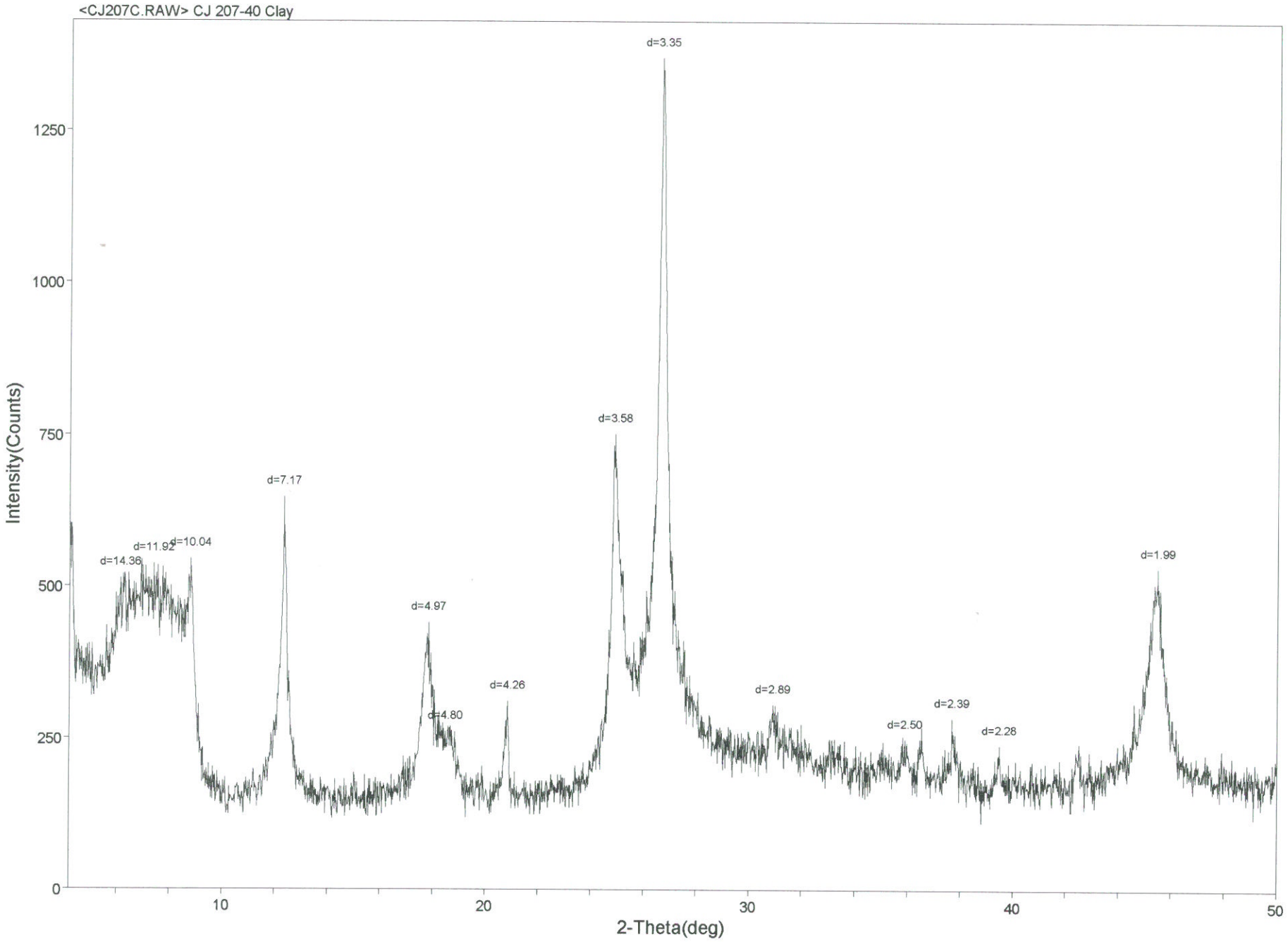

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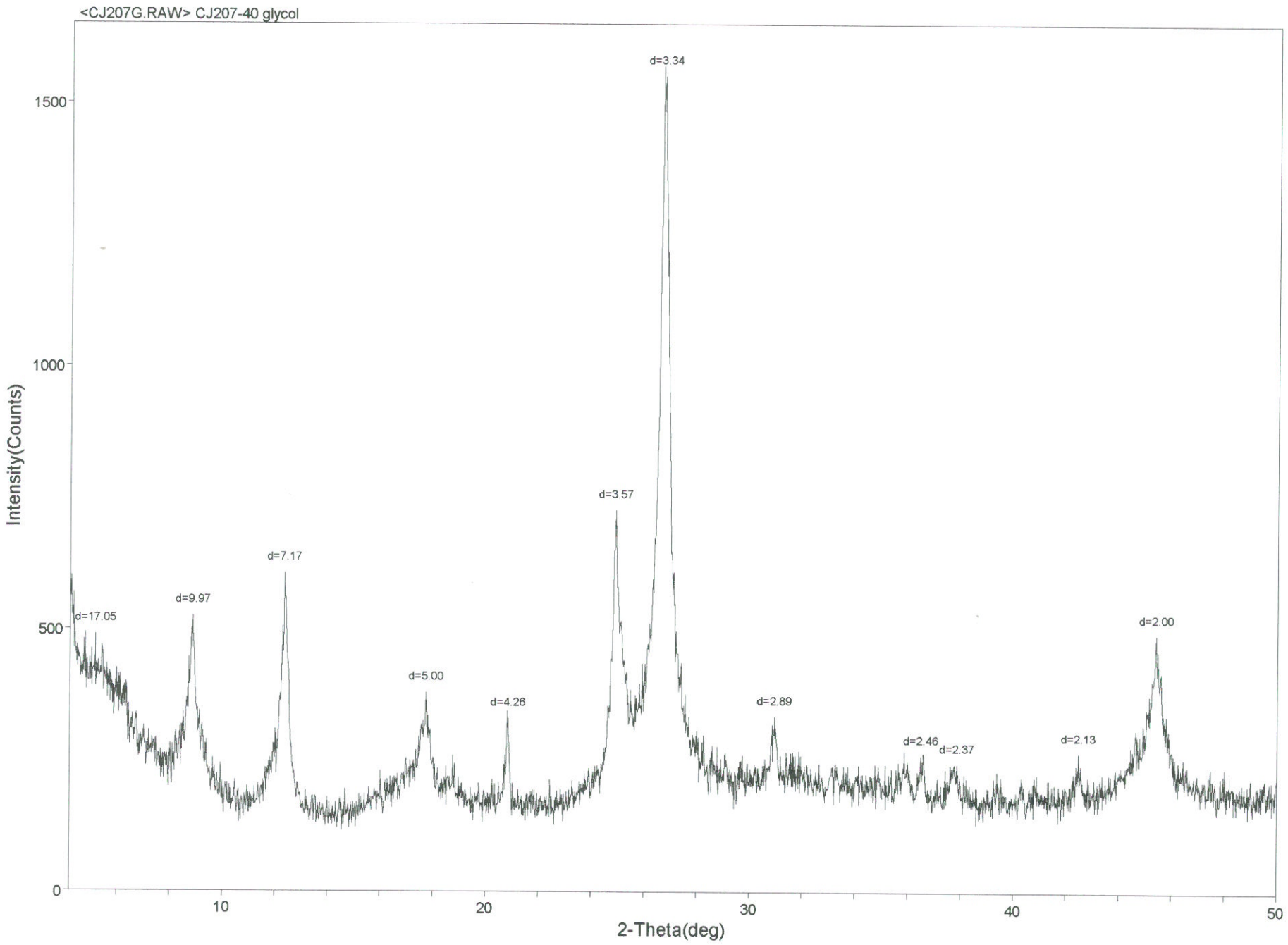

Mesa State College

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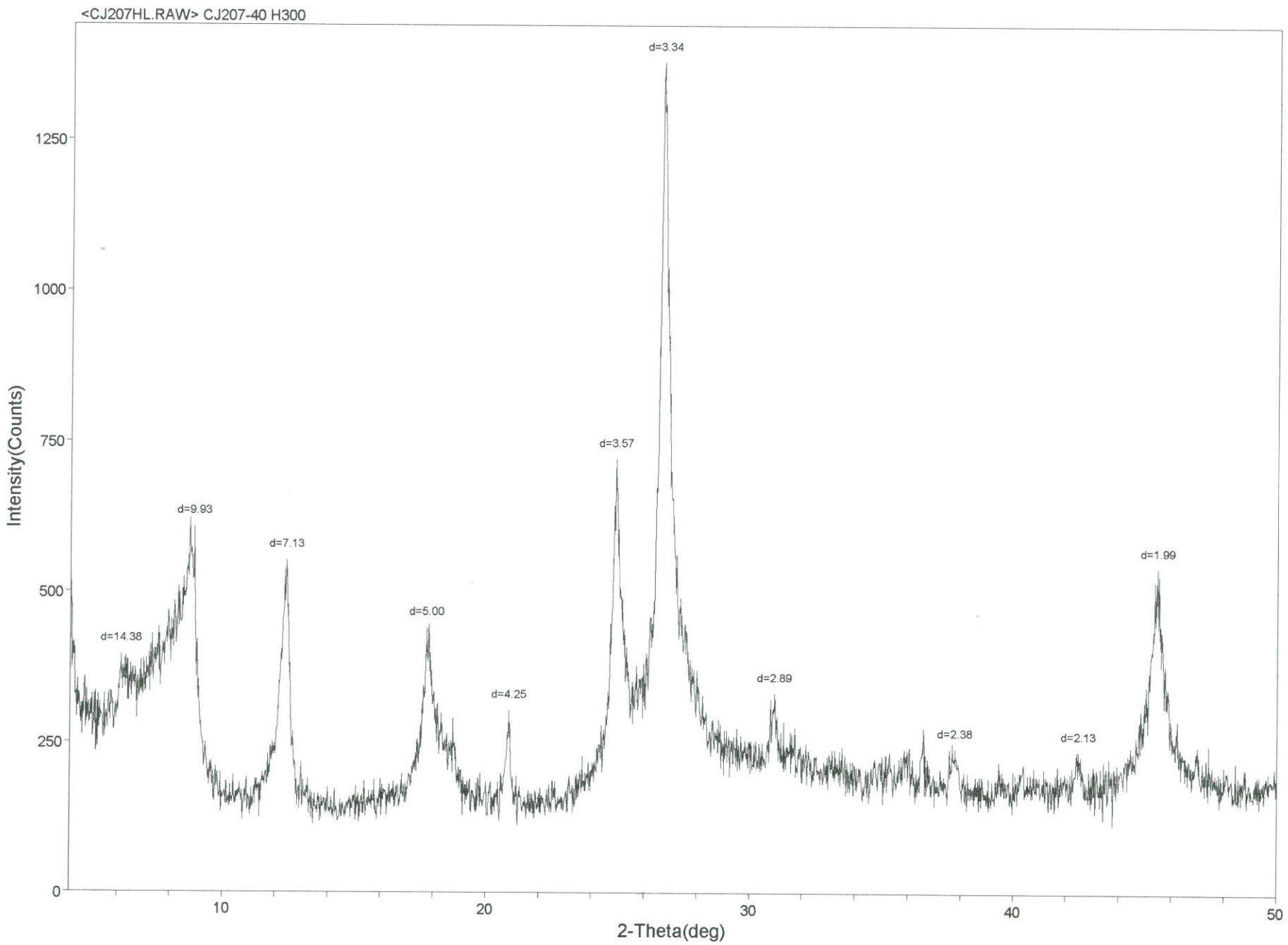

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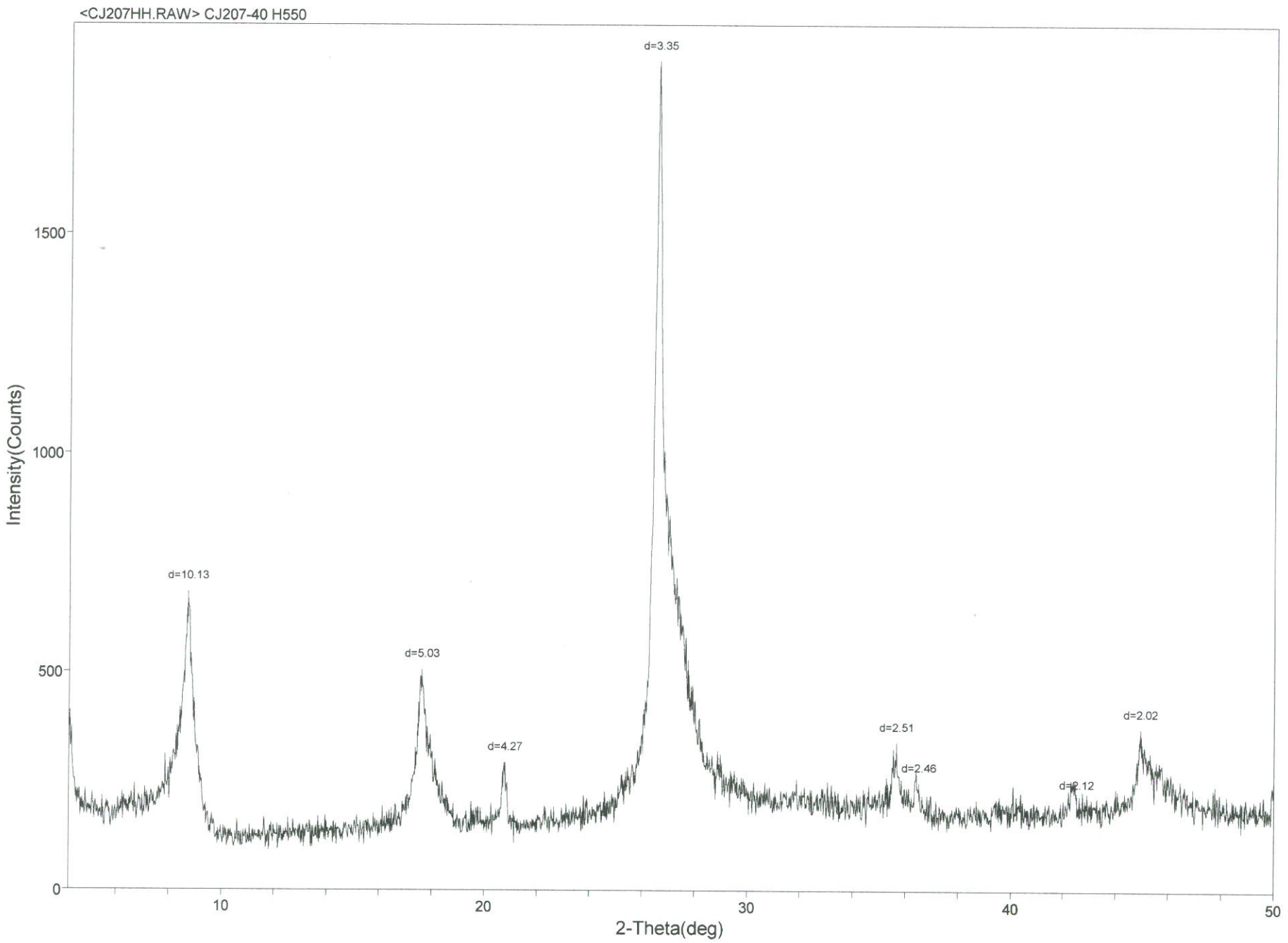

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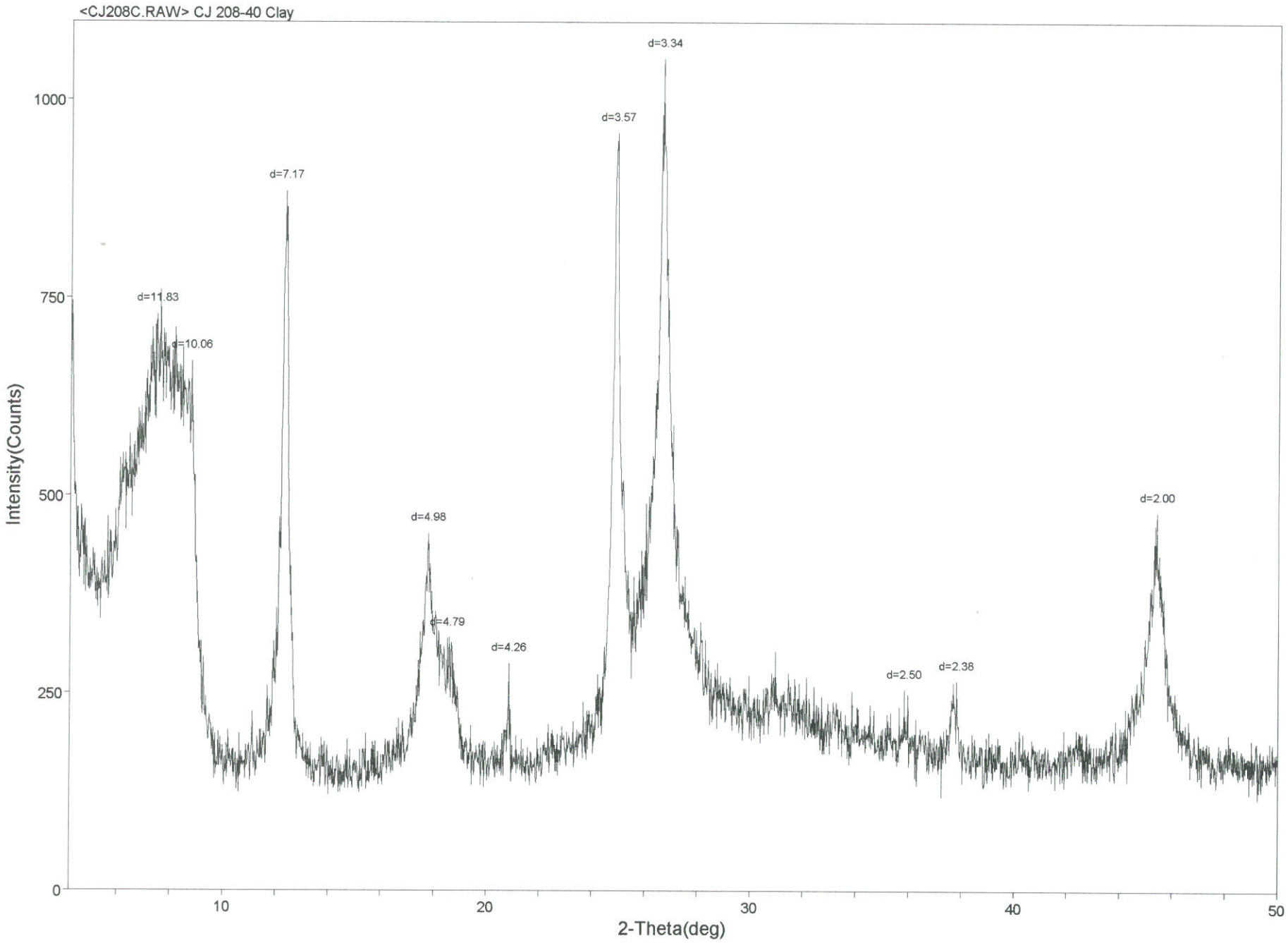

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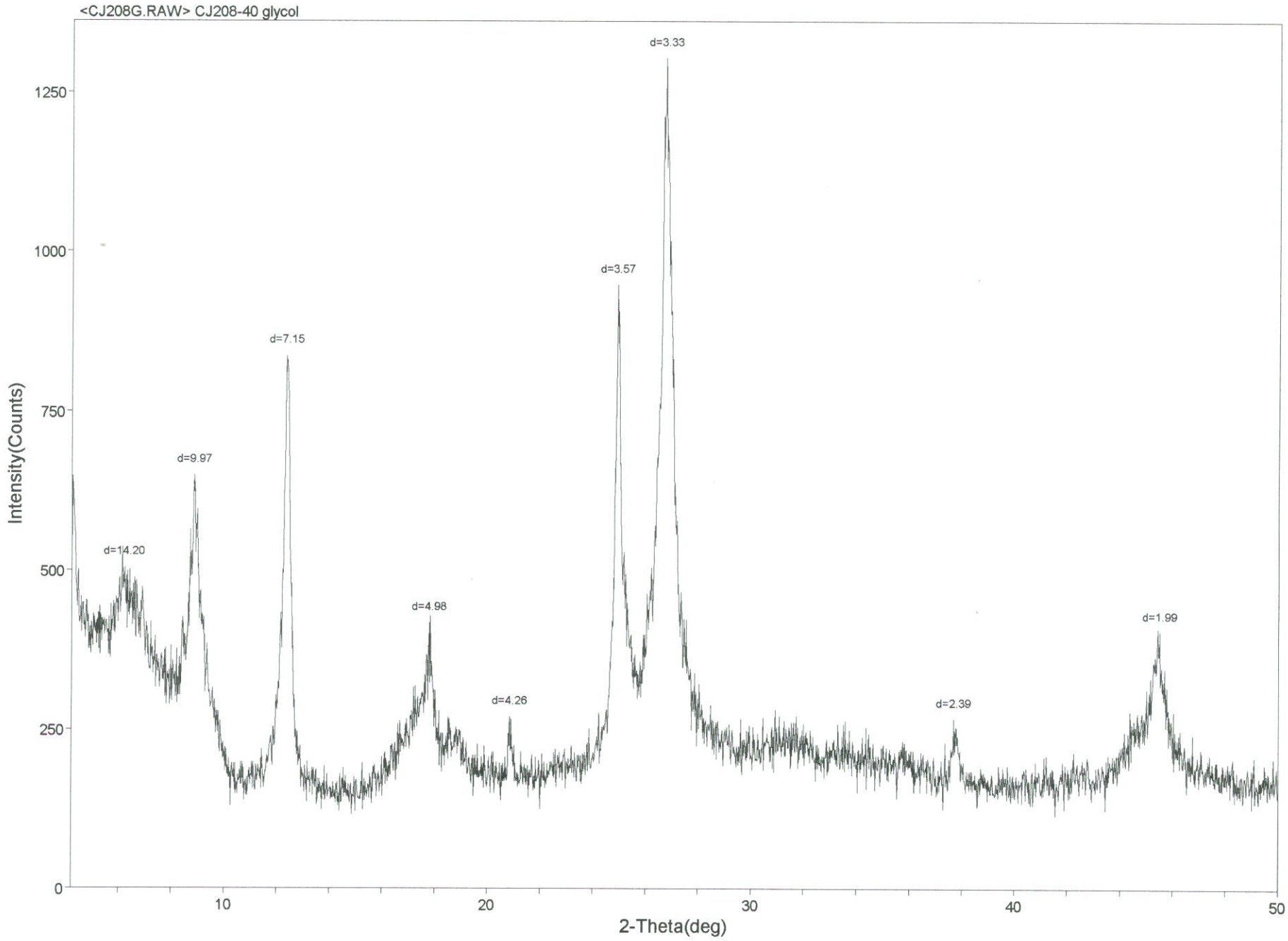

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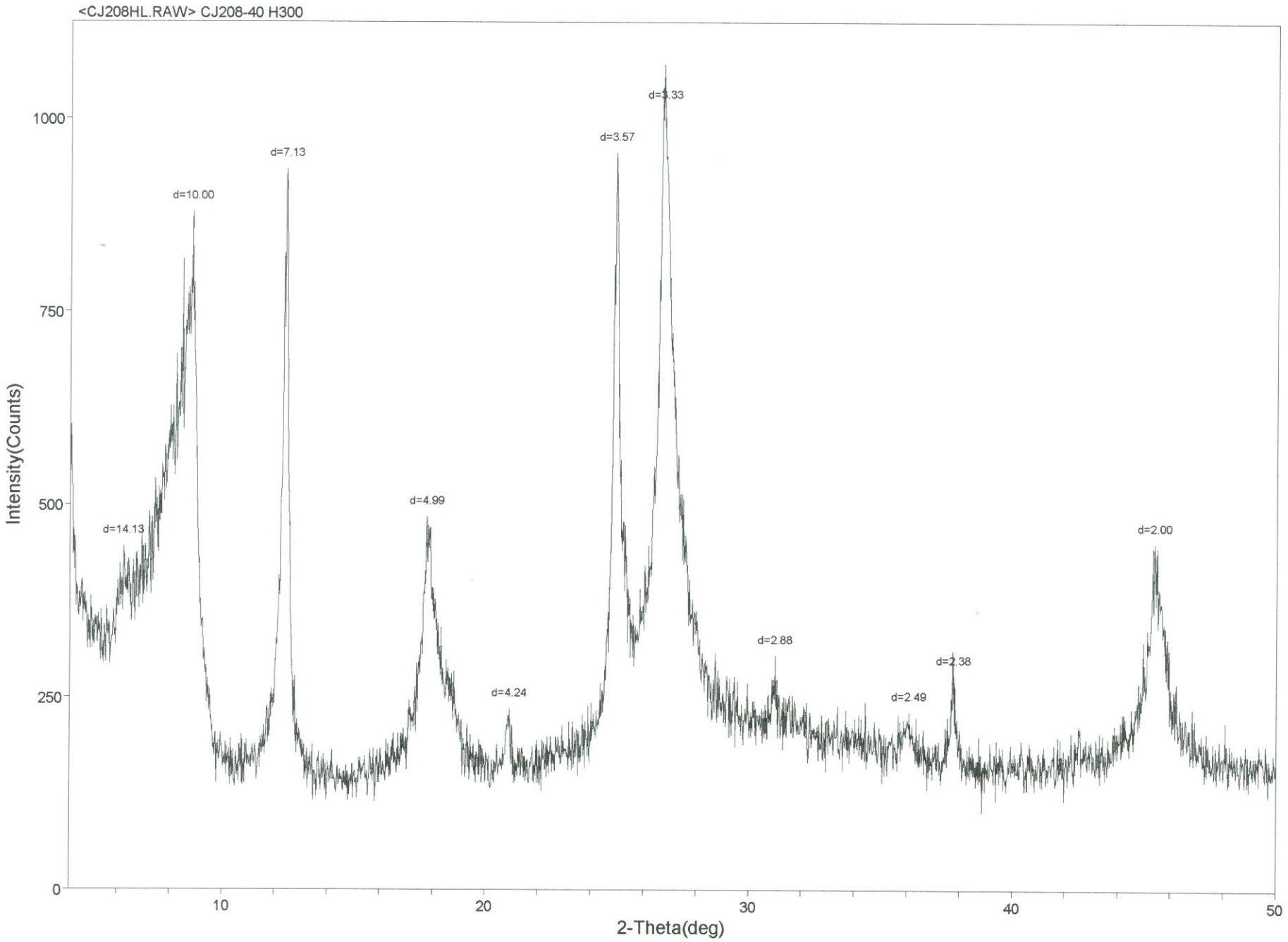

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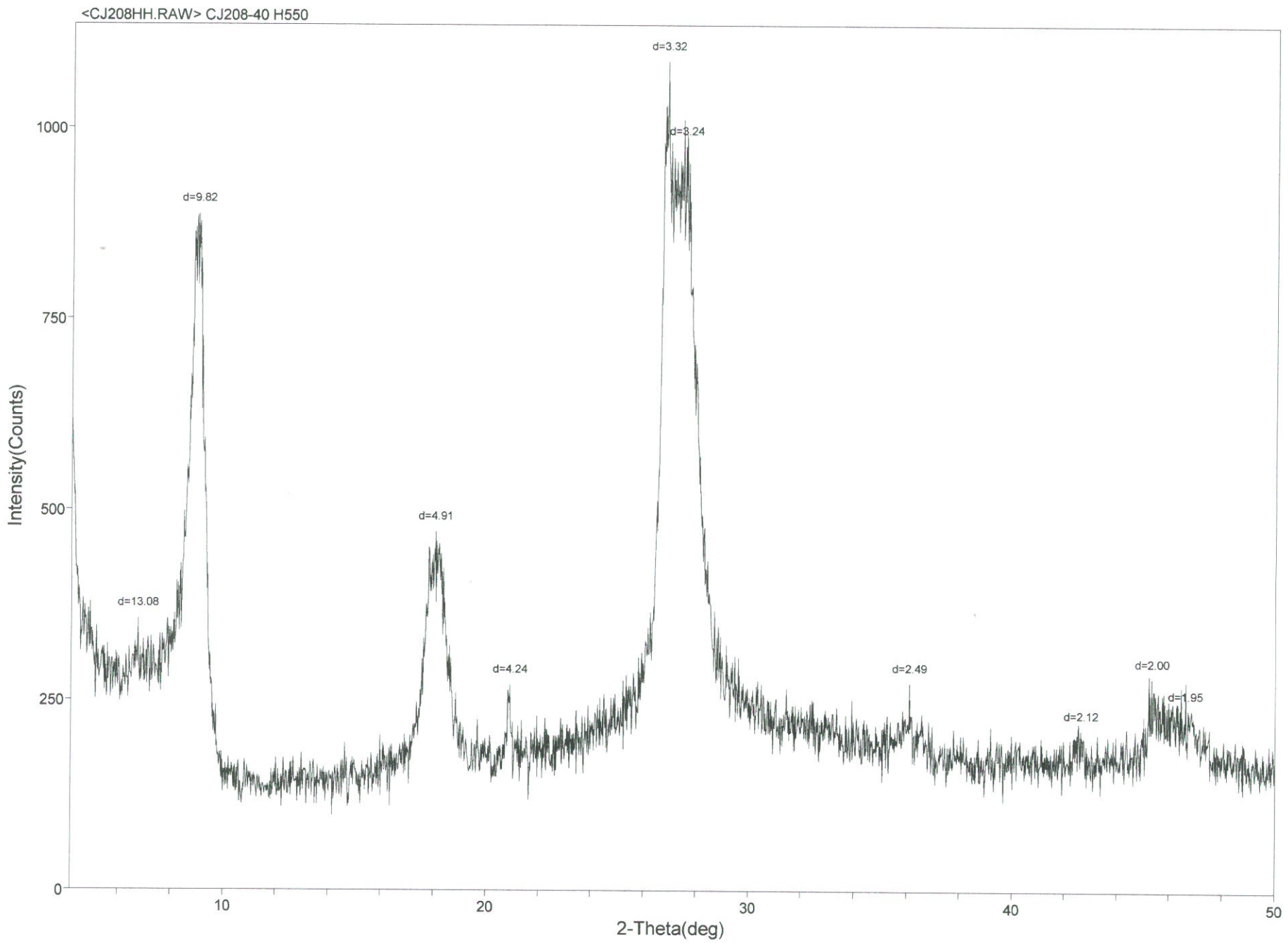

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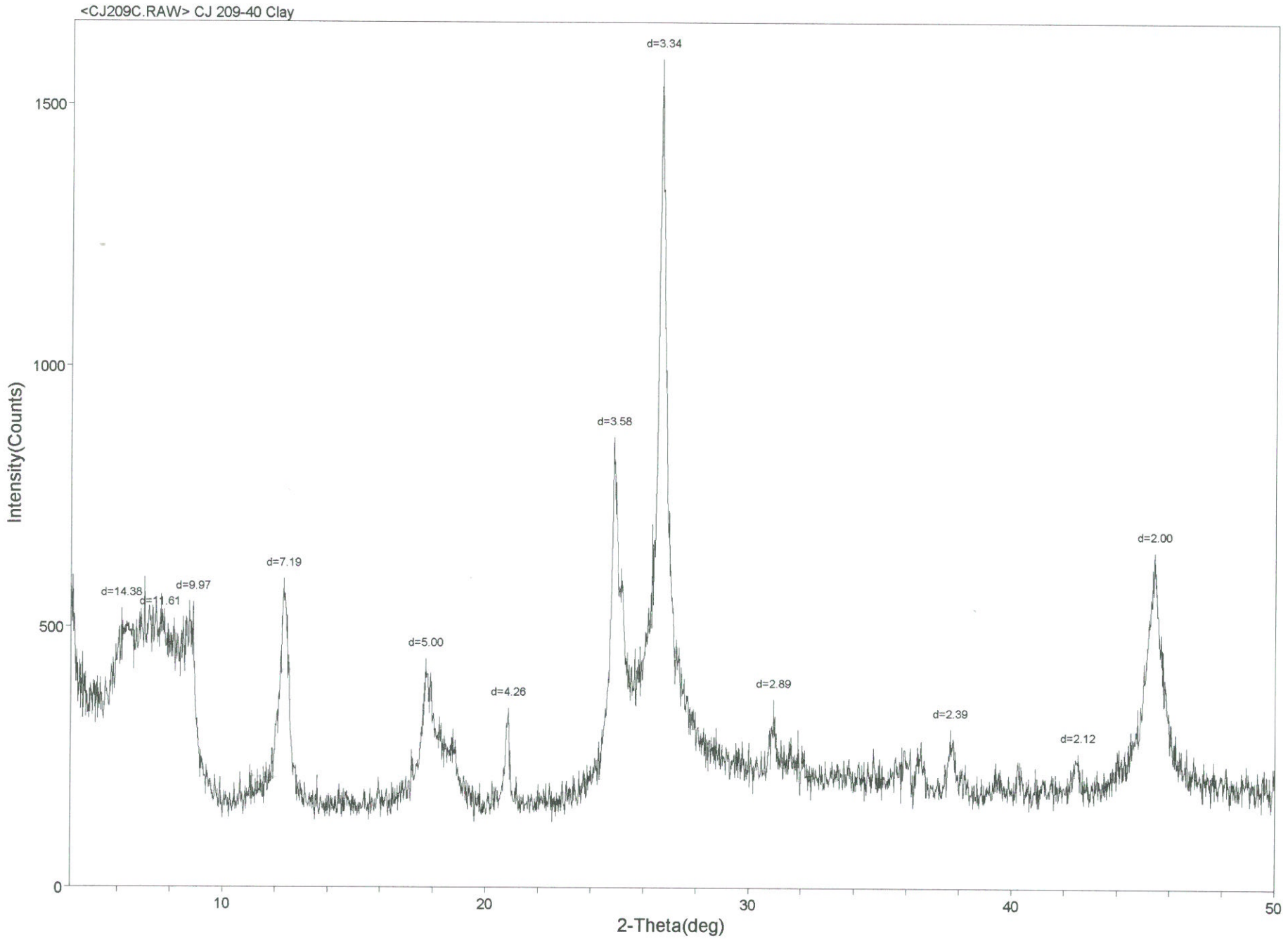

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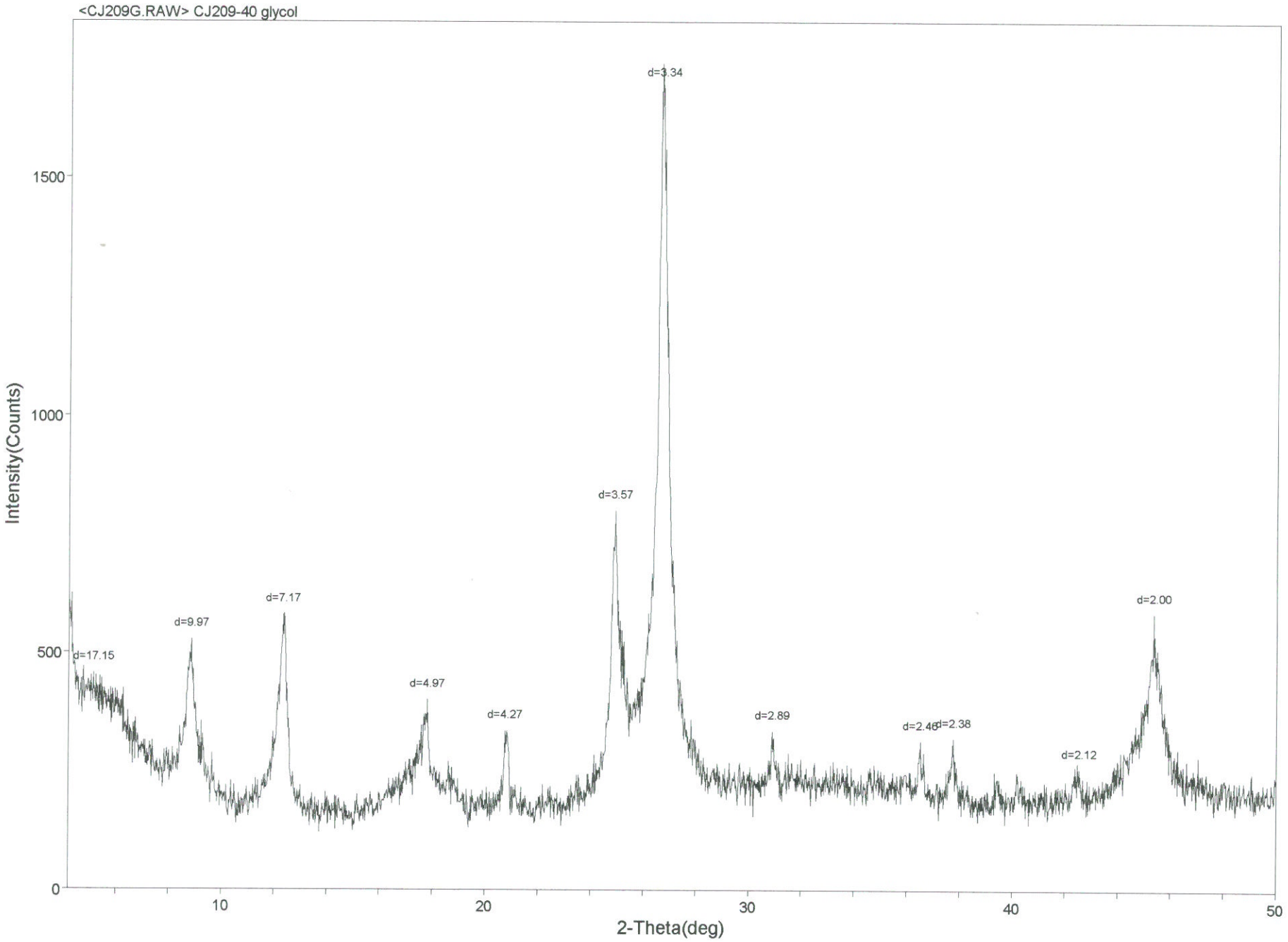

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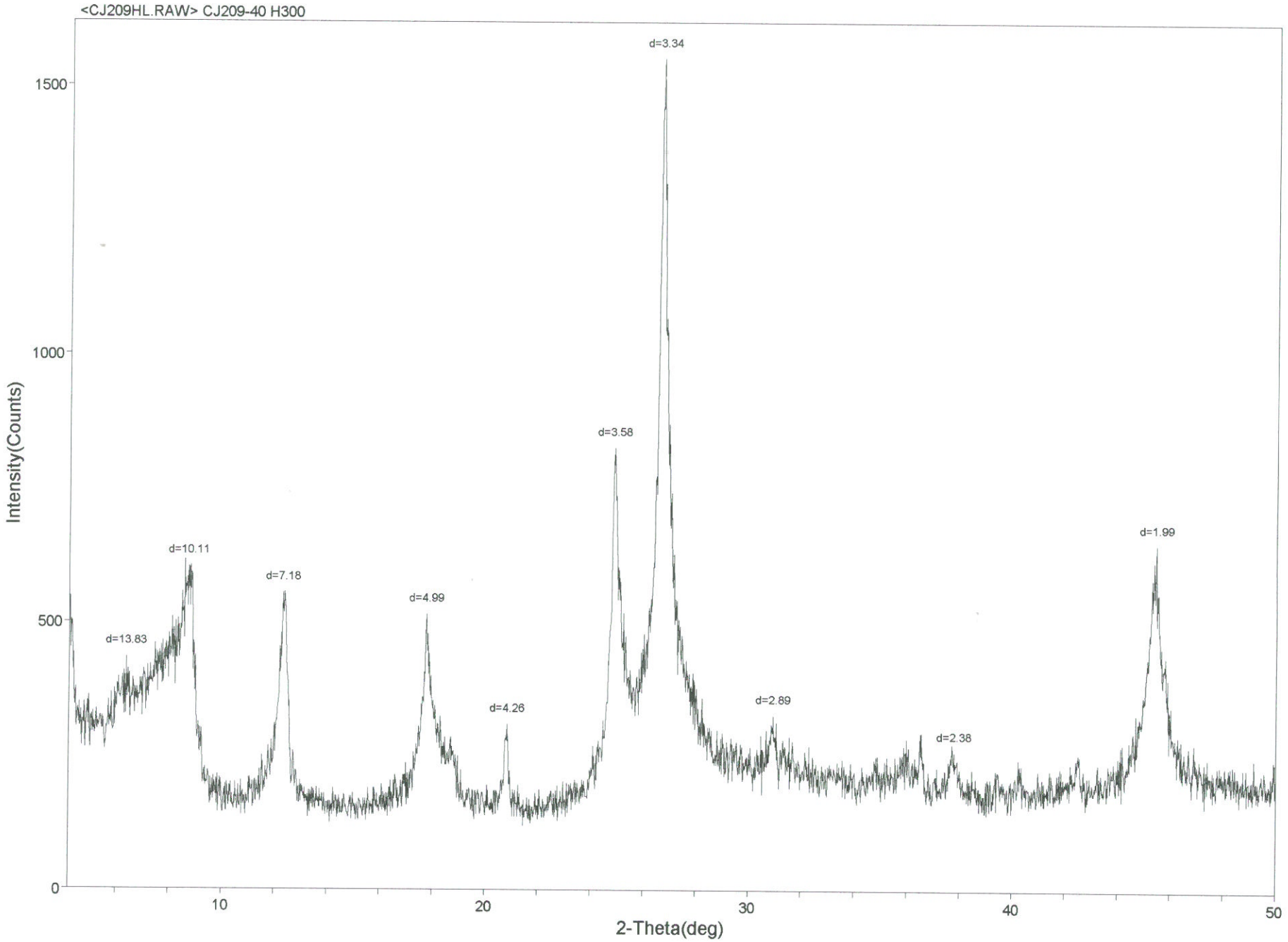

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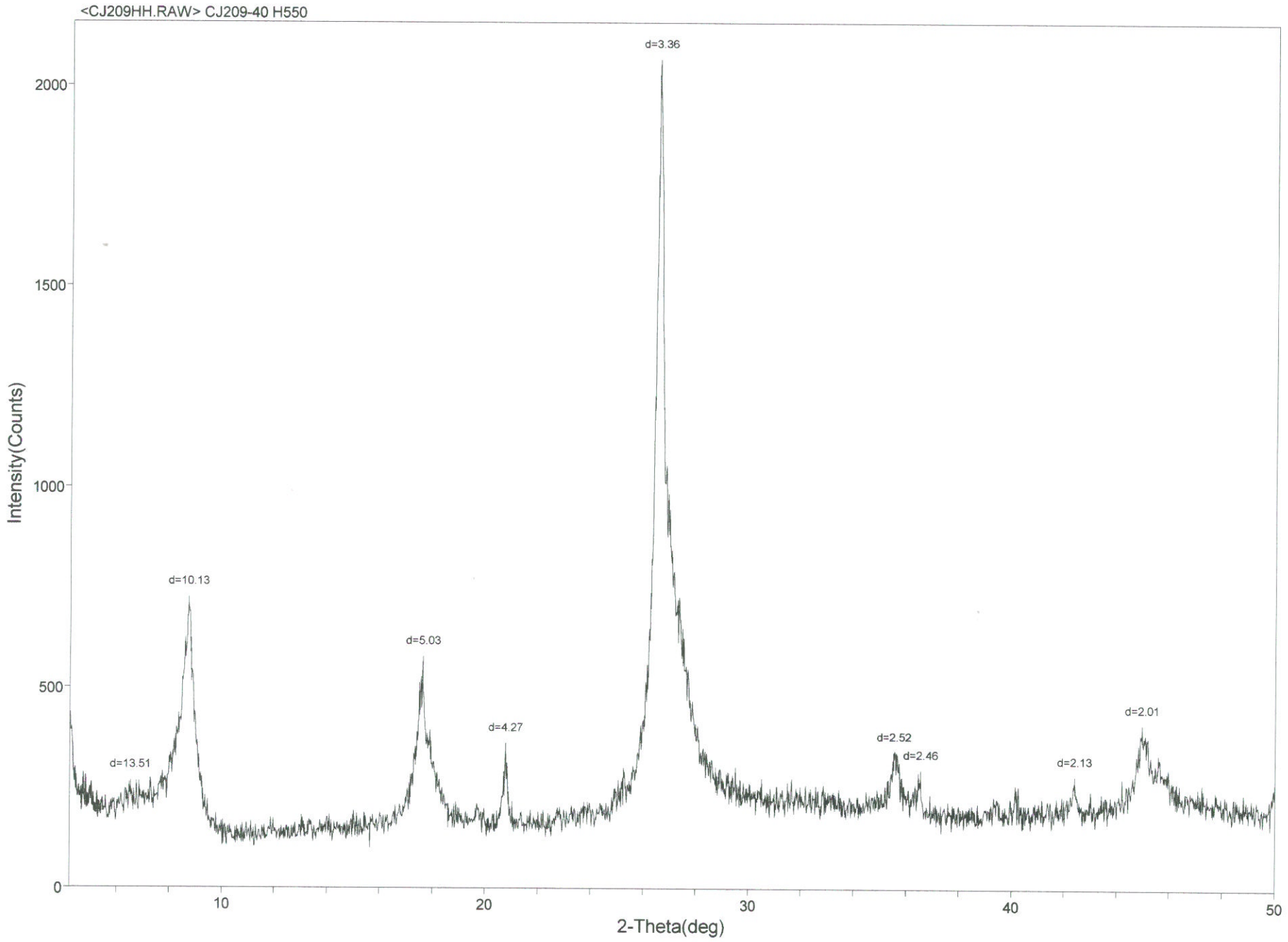

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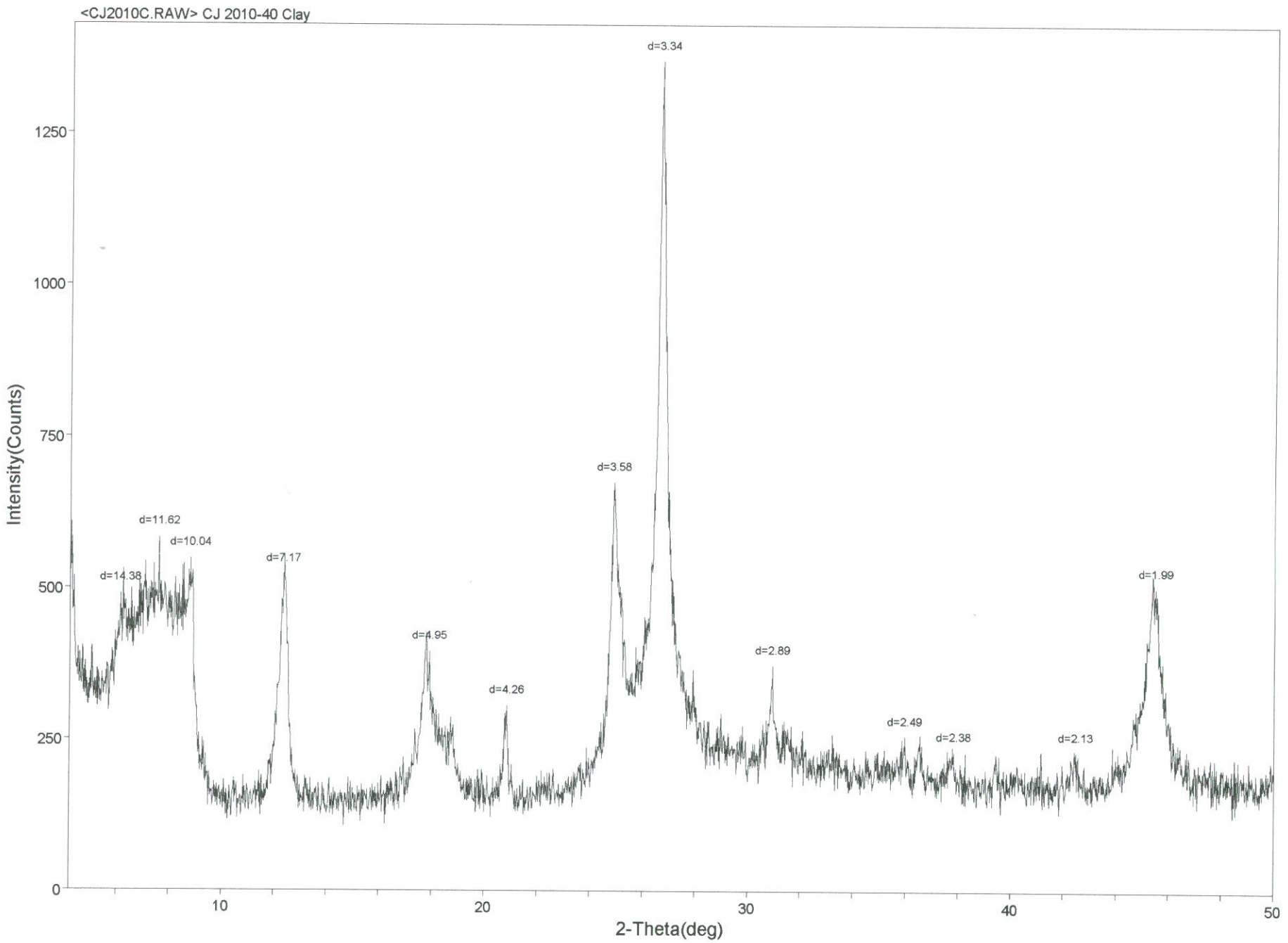

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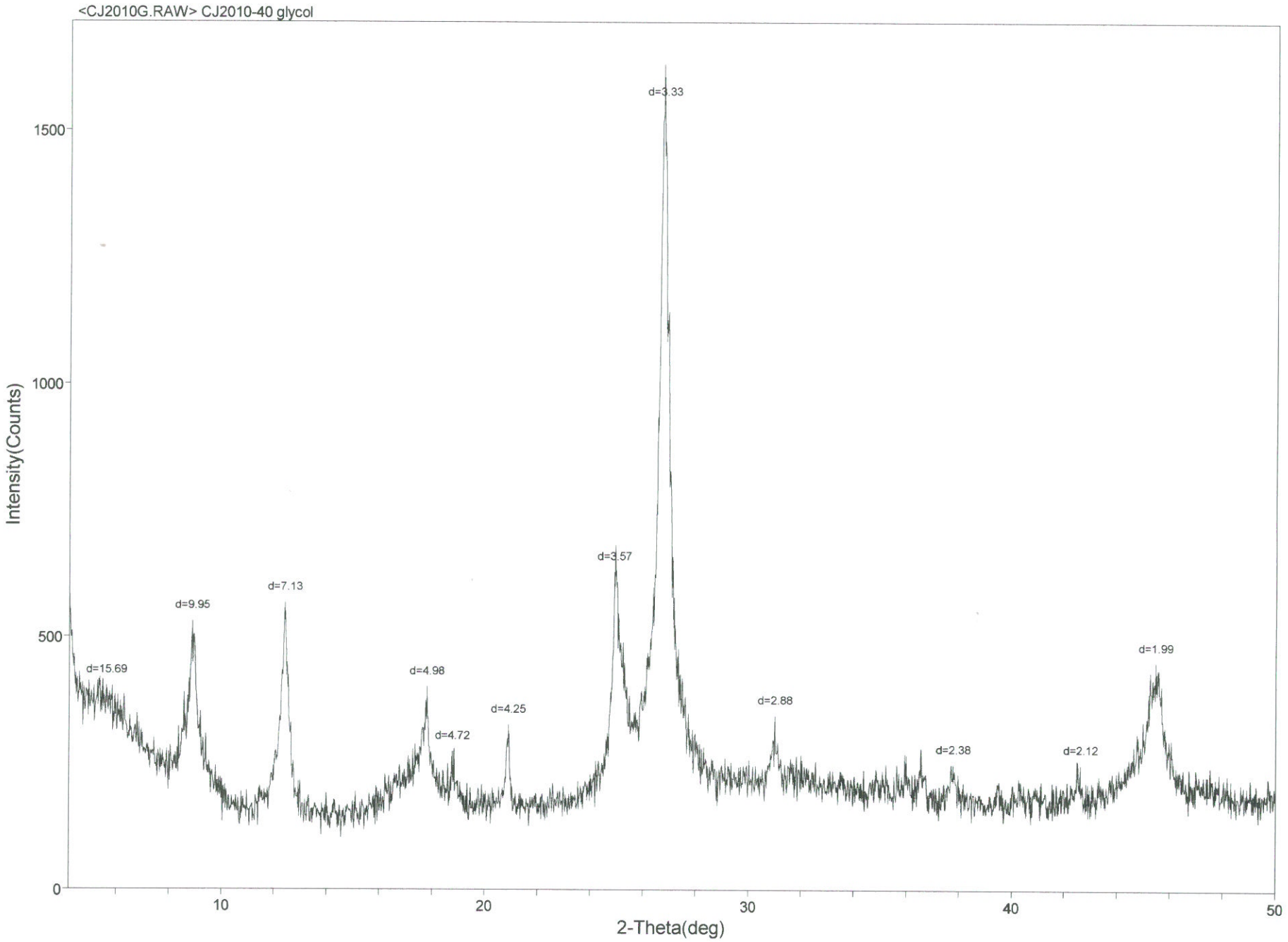

Mesa State College

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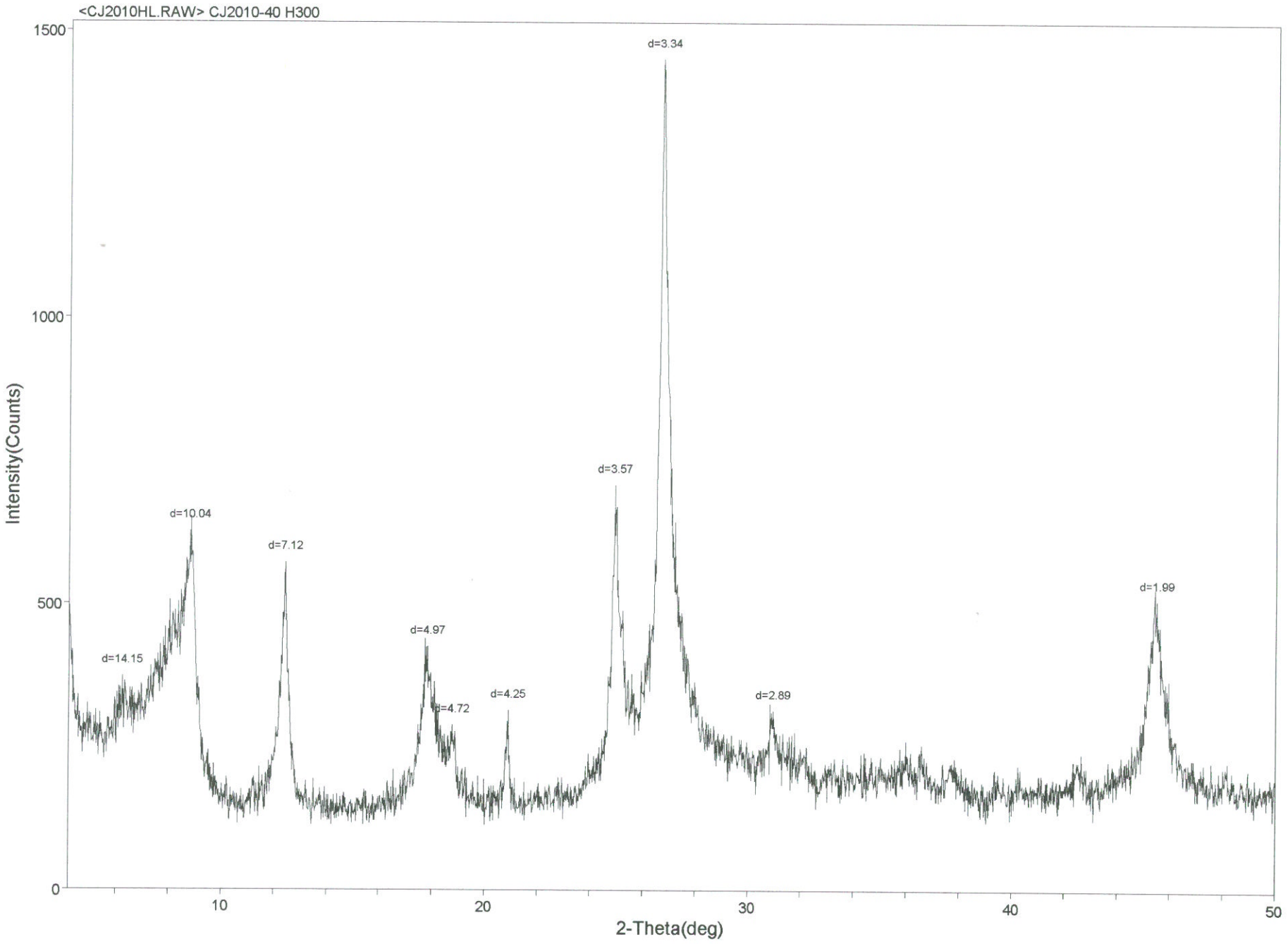

Mesa State College

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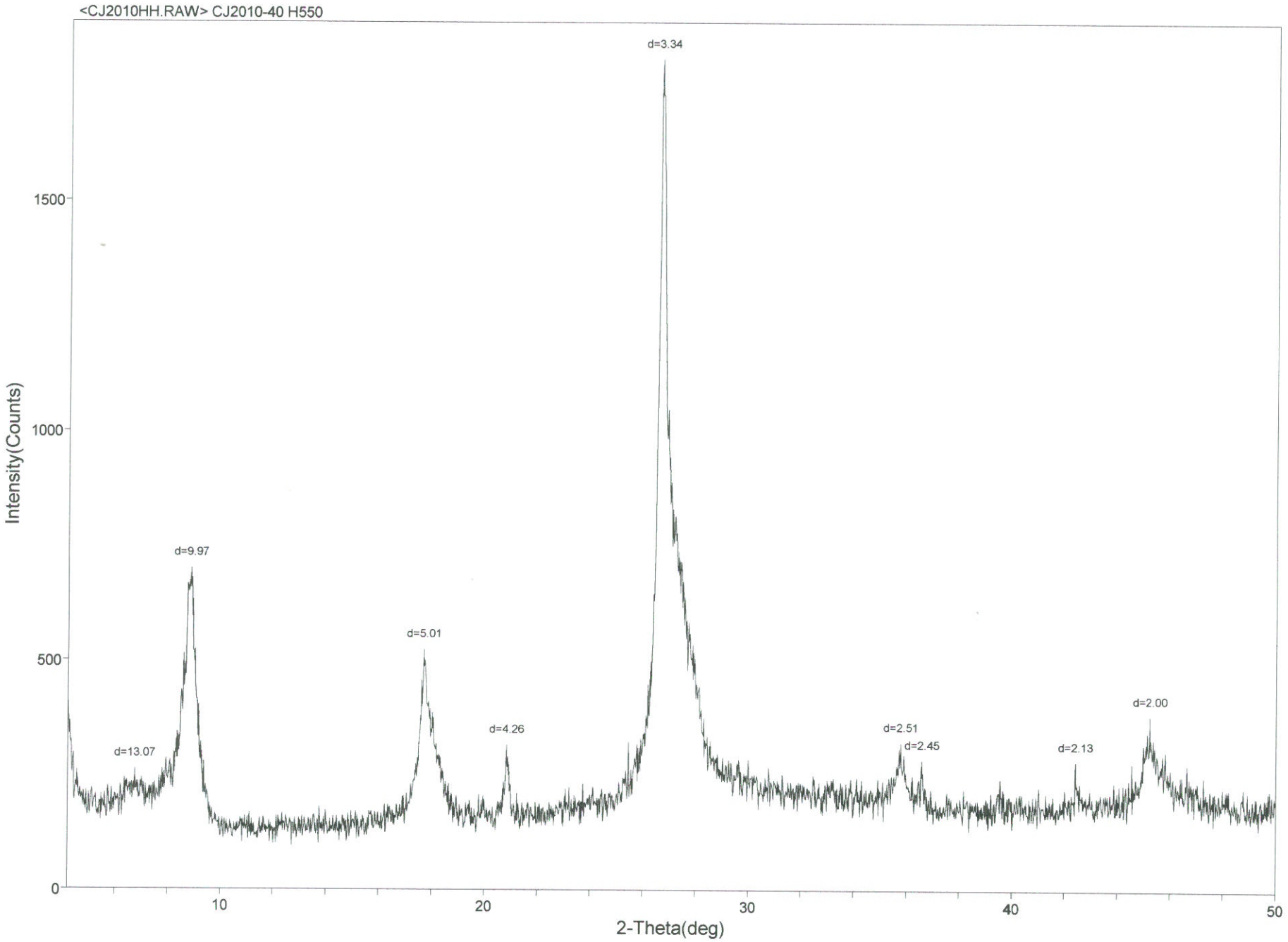

Mesa State College

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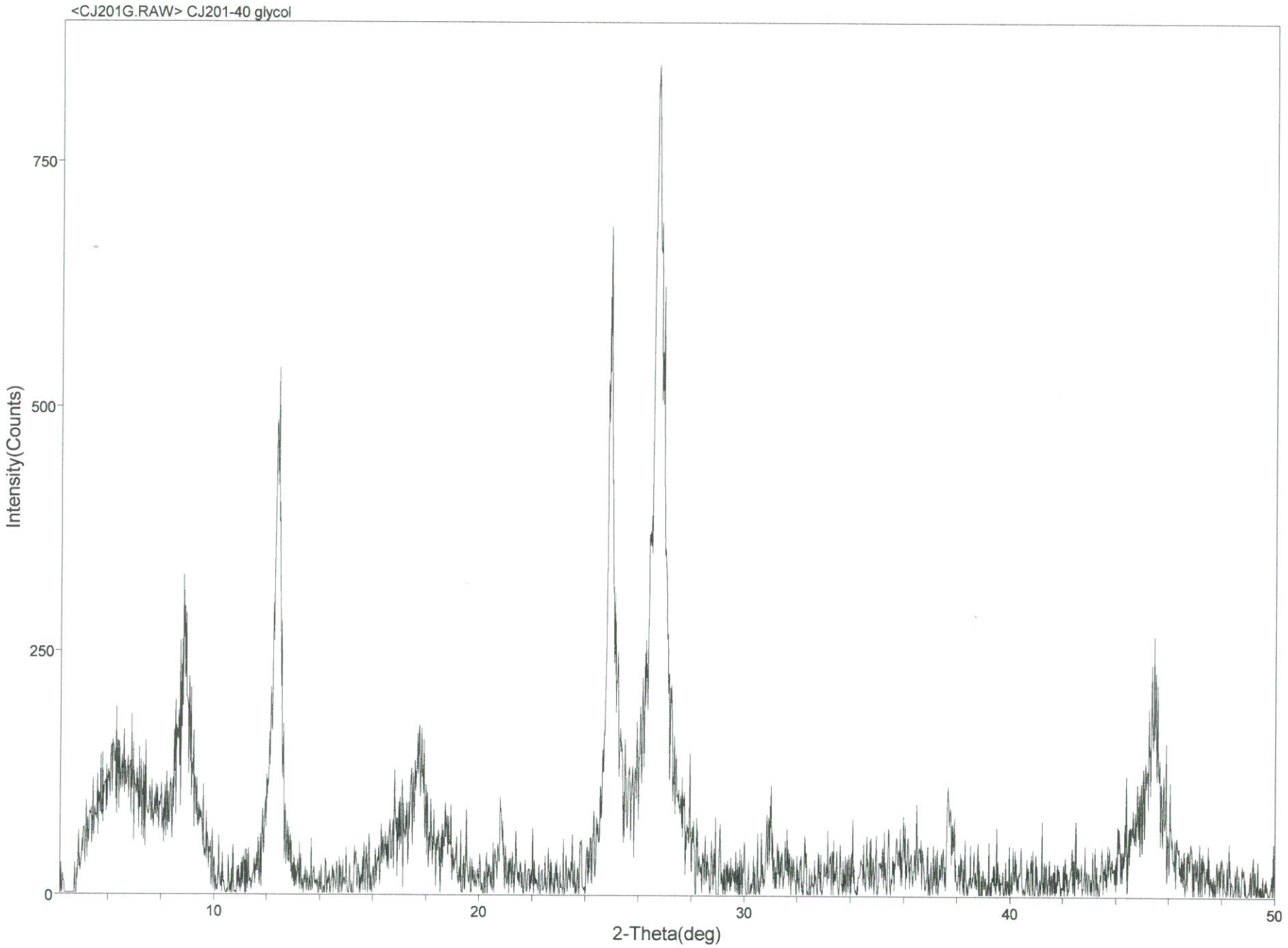
Appendix 7.

X-ray diffraction patterns of glycol solvated clays with background removed



Mesa State College

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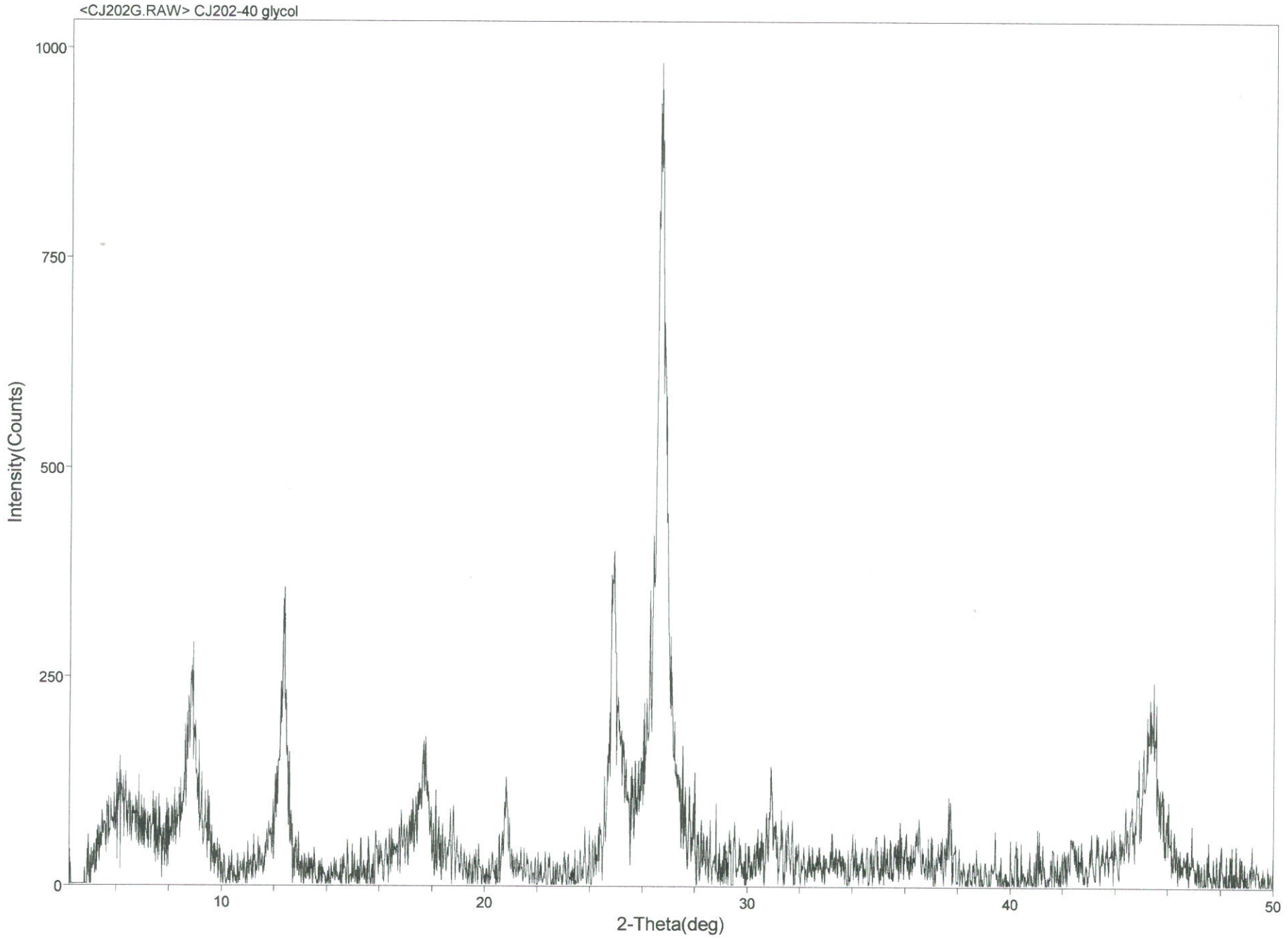

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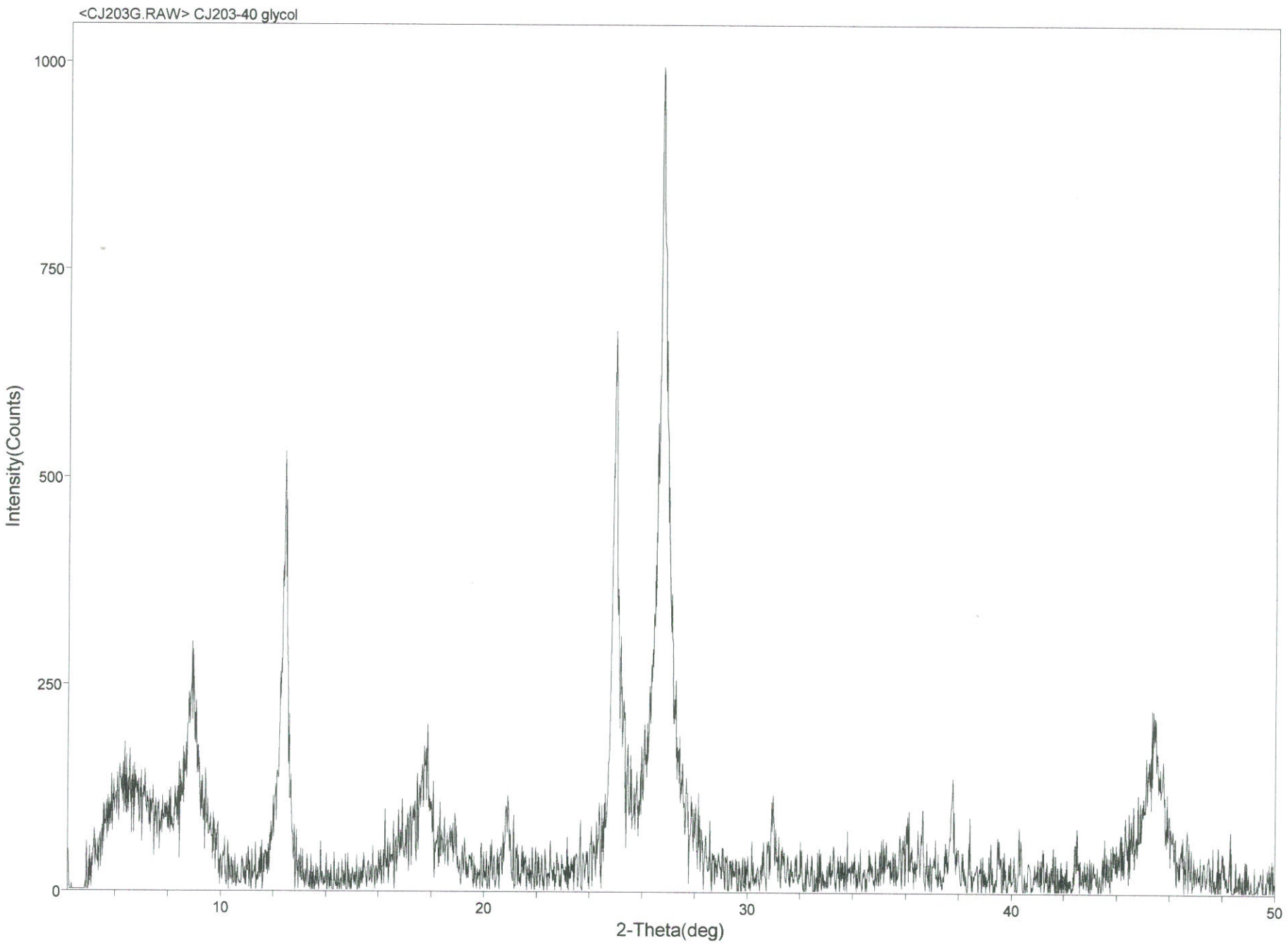

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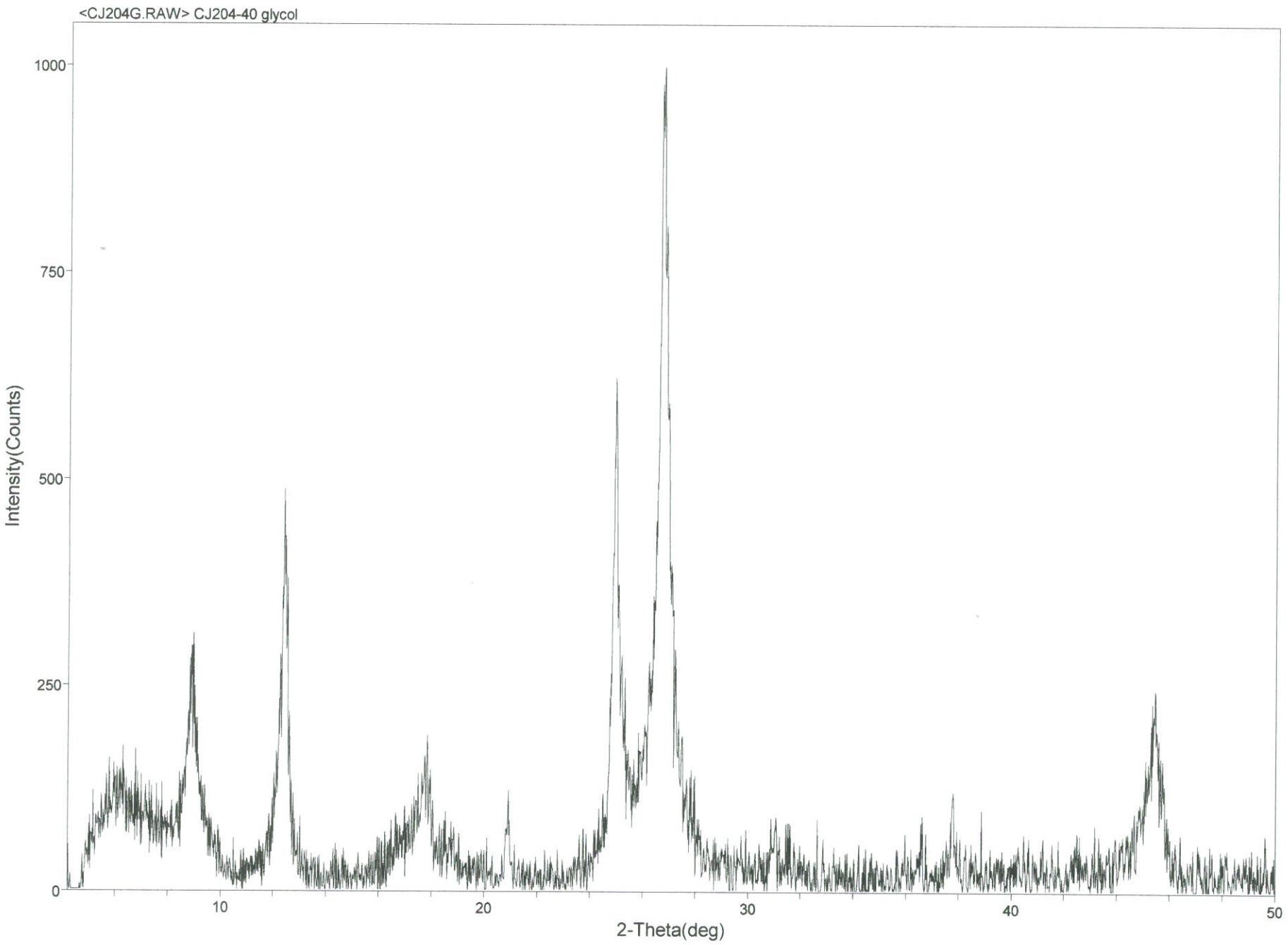

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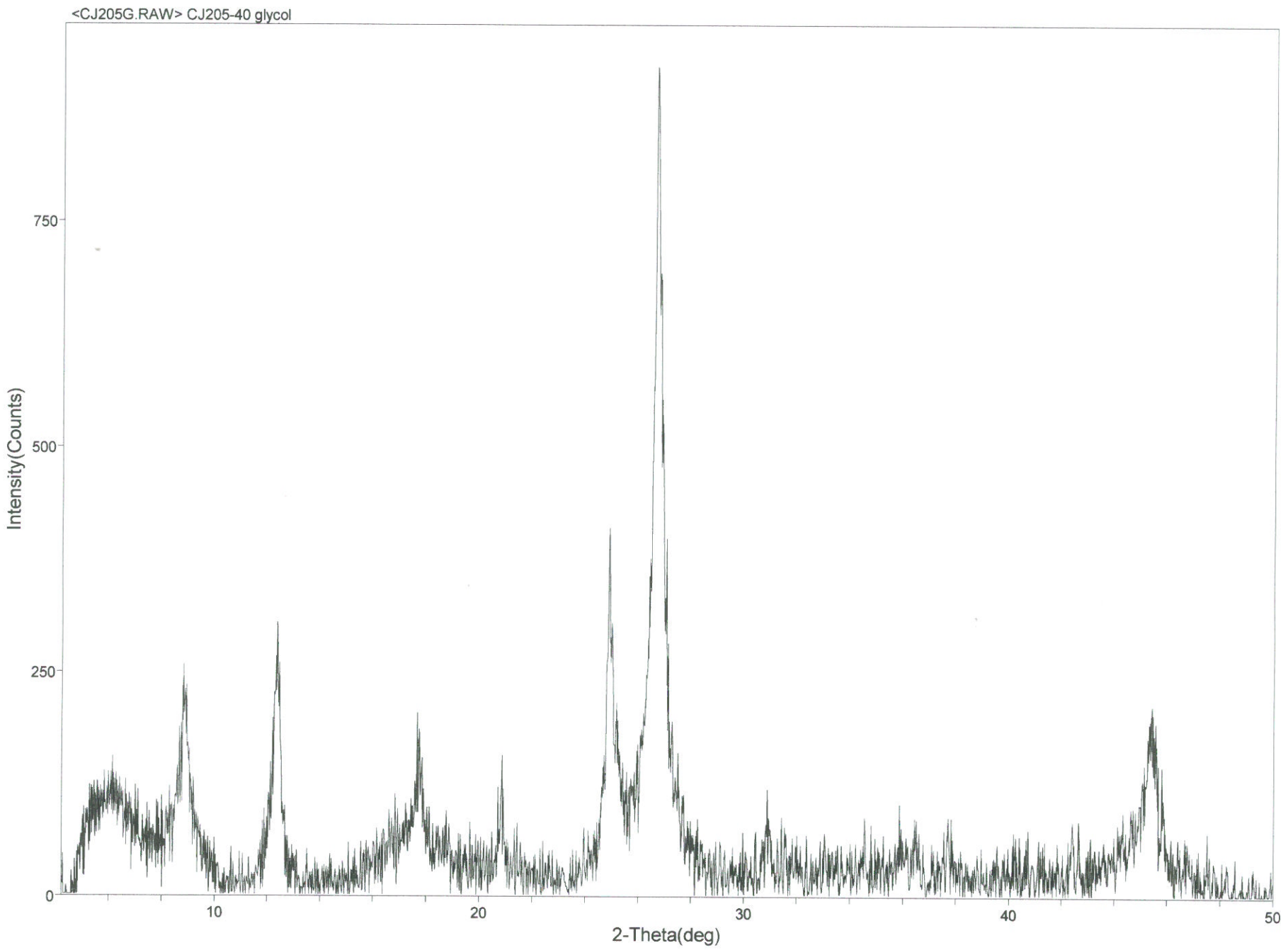

Mesa State College

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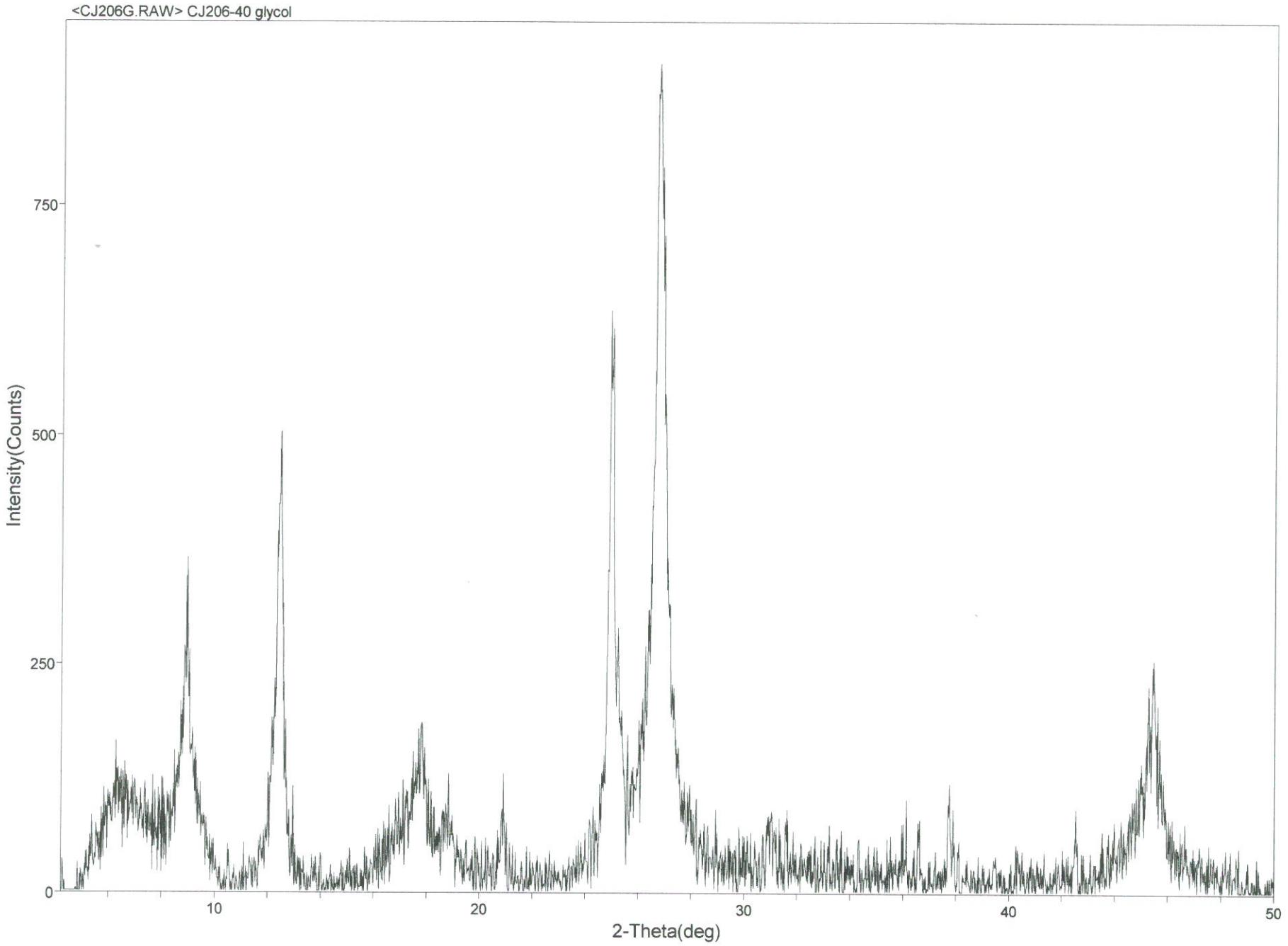
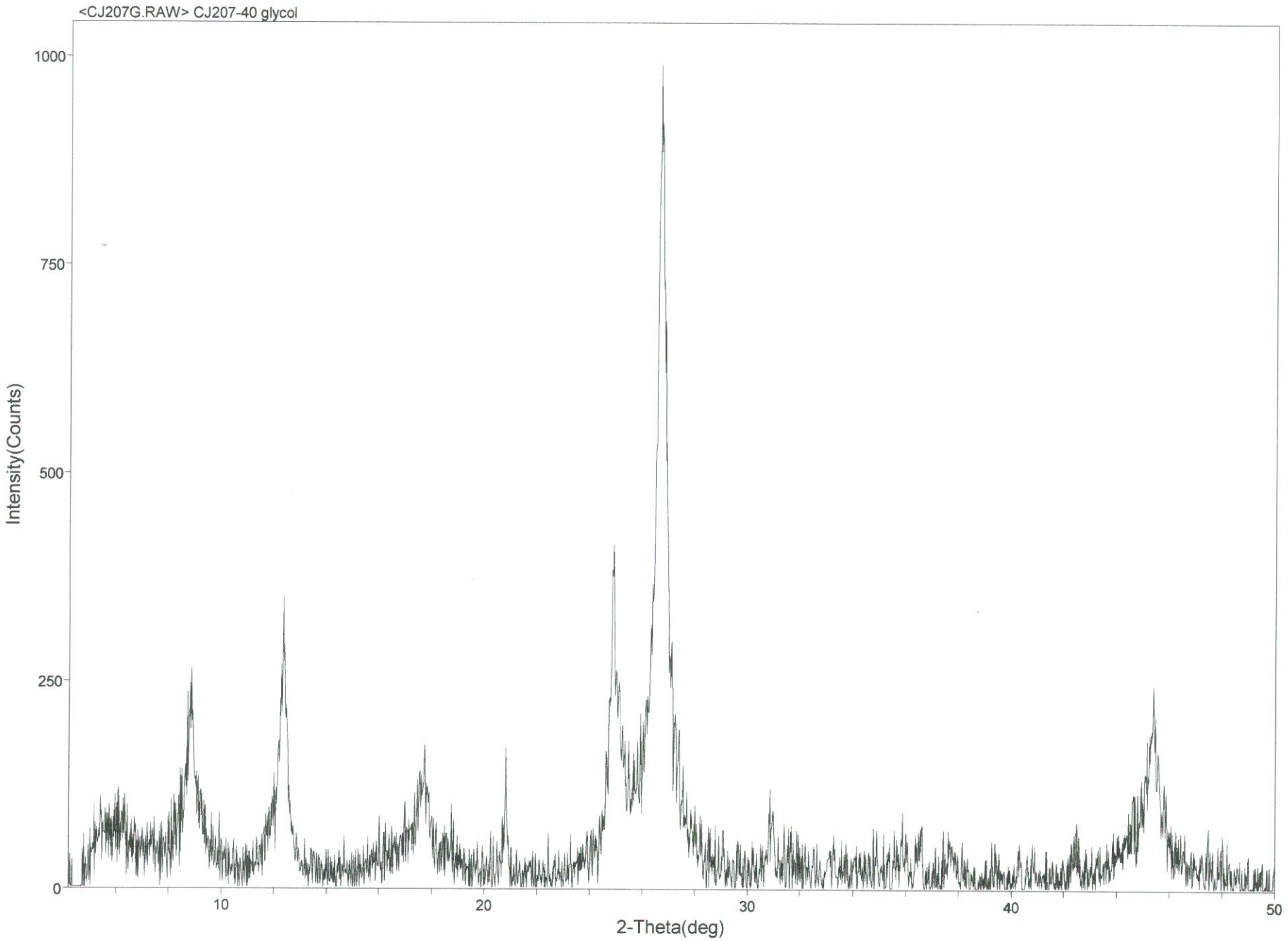


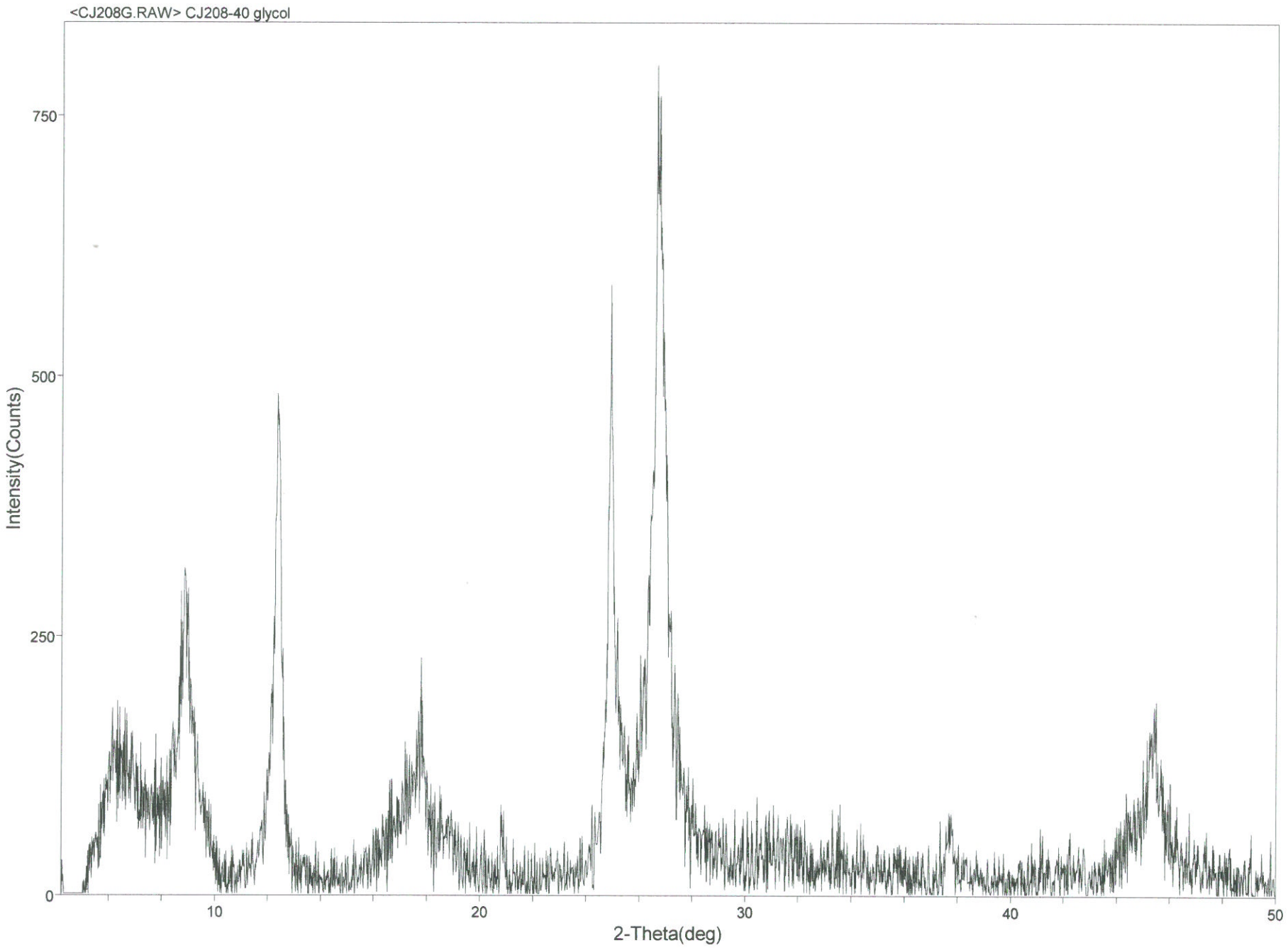
Mesa State College

<c:\hood\doe> Tuesday, Jan 31, 2006 @03:07p



Mesa State College

<c:\hood\doe> Tuesday, Jan 31, 2006 @03:10p



Mesa State College

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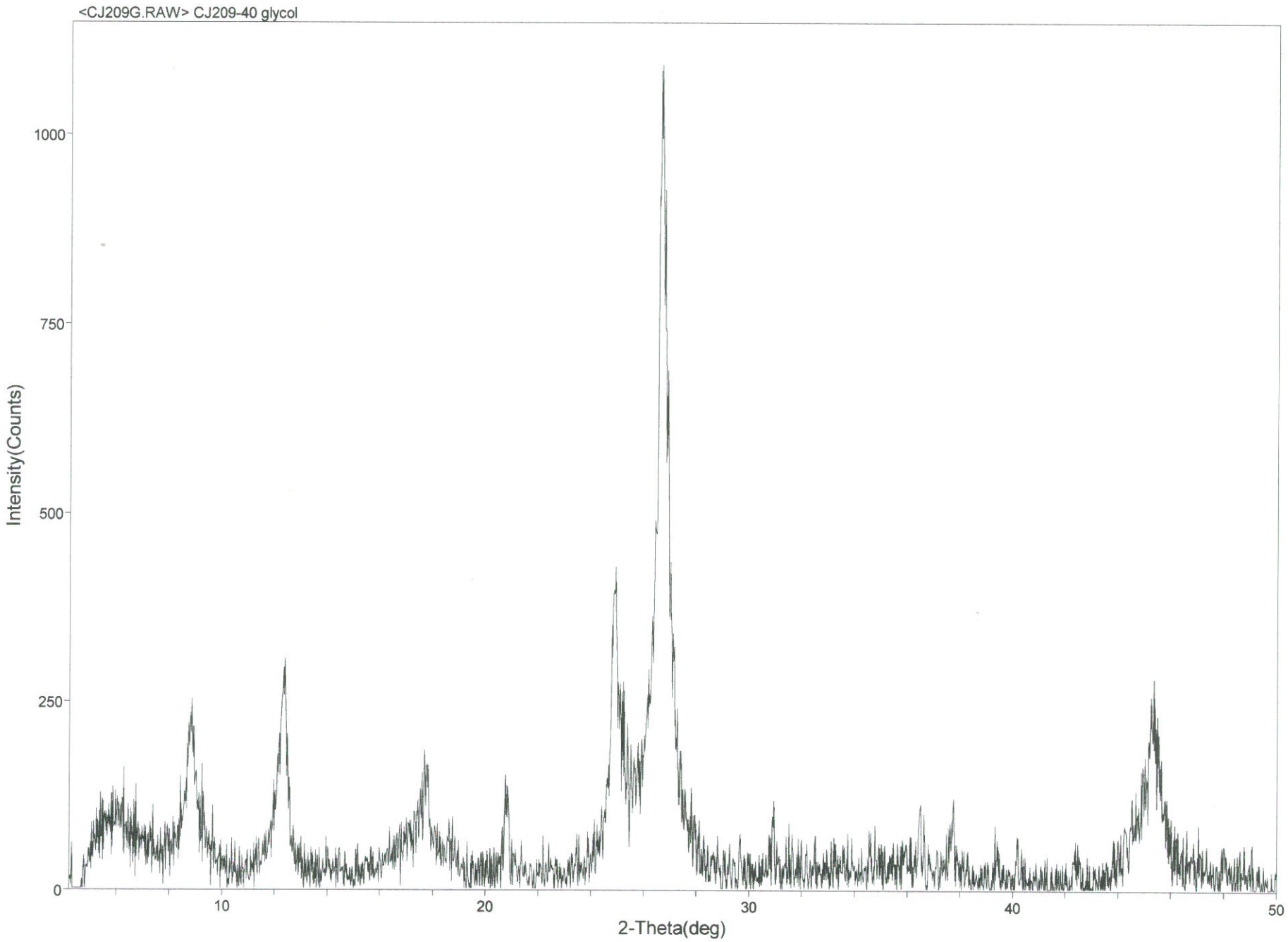
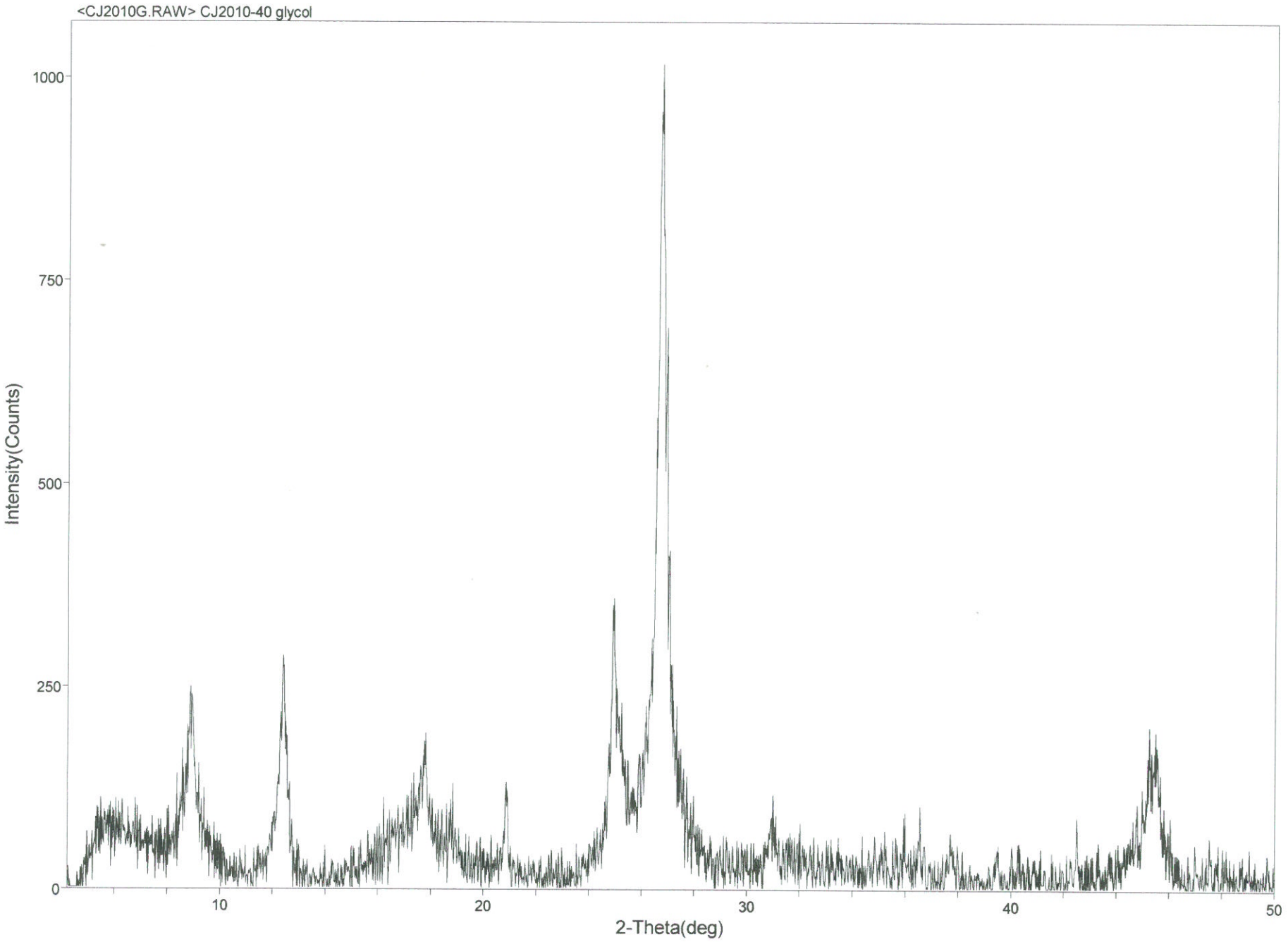


Mesa State College

<c:\hood\doe> Tuesday, Jan 31, 2006 @03:15p



Mesa State College

<c:\hood\doe> Tuesday, Jan 31, 2006 @03:17p

Appendix E

Copies of Analytical Reports of BET Surface Area Analysis

Prepared by Micromeritics Analytical Services
Norcross, Georgia

Sample: CJ-201-40 06-0210 3/3
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0210.SMP

Started: 2/1/2006 12:27:55PM
Completed: 2/1/2006 3:23:59PM
Report Time: 2/1/2006 3:24:00PM
Warm Free Space: 5.1716 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.2757 g
Cold Free Space: 14.2717 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Tabular Report

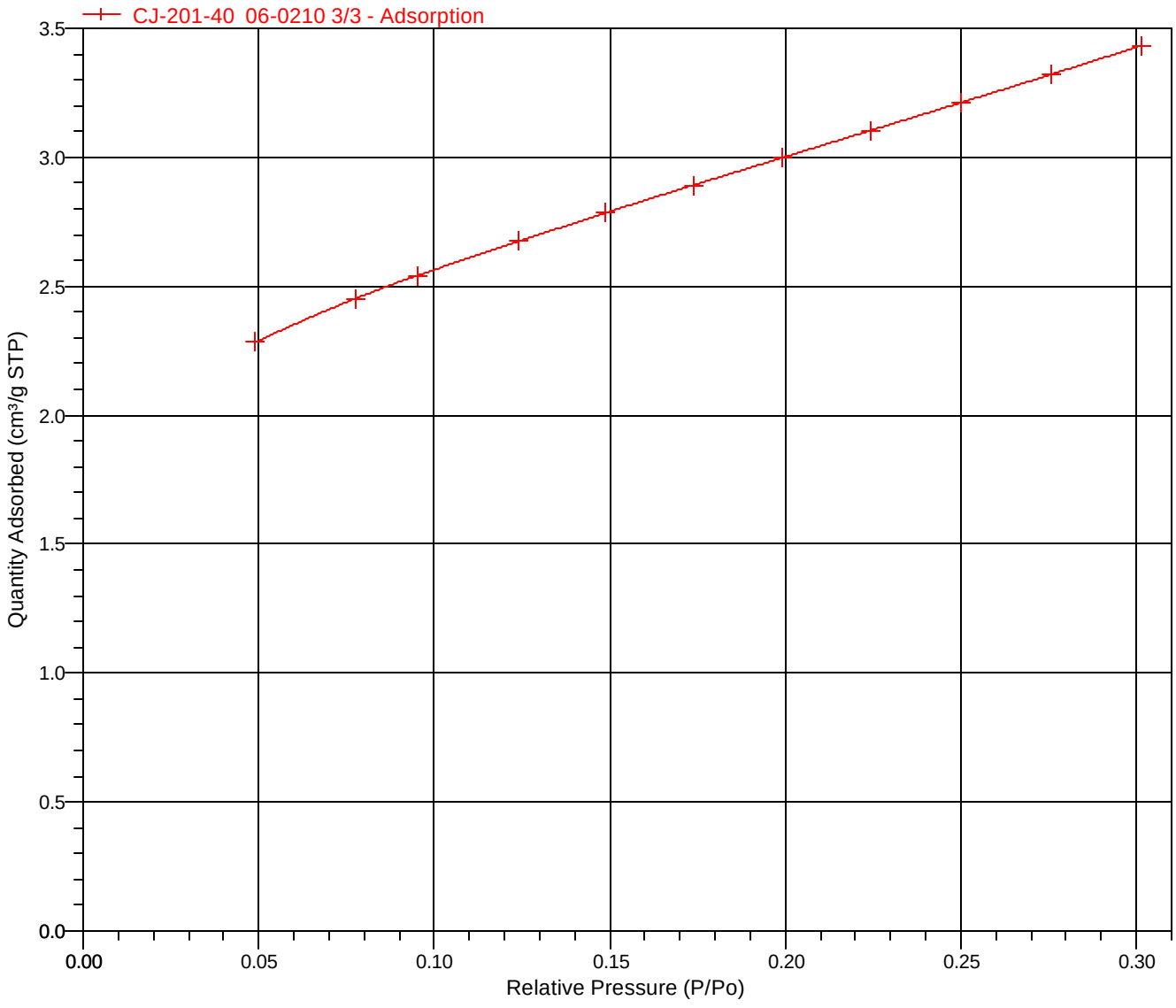
Relative Pressure (P/Po)	Absolute Pressure (mmHg)	Quantity Adsorbed (cm³/g STP)	Elapsed Time (h:min)	Saturation Pressure (mmHg)
			01:10	735.79211
0.048910454	35.98793	2.2822	01:49	
0.077386655	56.94049	2.4522	01:59	
0.095083473	69.96167	2.5421	02:08	
0.123883388	91.15242	2.6734	02:15	
0.148628264	109.35950	2.7840	02:22	
0.173850205	127.91761	2.8924	02:28	
0.199214129	146.58018	2.9983	02:33	
0.224543969	165.21768	3.1044	02:39	
0.250010120	183.95547	3.2120	02:44	
0.275550098	202.74759	3.3213	02:50	
0.301305895	221.69850	3.4329	02:55	

Sample: CJ-201-40 06-0210 3/3
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0210.SMP

Started:	2/1/2006 12:27:55PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 3:23:59PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 3:24:00PM	Sample Mass:	4.2757 g
Warm Free Space:	5.1716 cm³ Measured	Cold Free Space:	14.2717 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Linear Plot



Sample: CJ-201-40 06-0210 3/3
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0210.SMP

Started: 2/1/2006 12:27:55PM
Completed: 2/1/2006 3:23:59PM
Report Time: 2/1/2006 3:24:00PM
Warm Free Space: 5.1716 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.2757 g
Cold Free Space: 14.2717 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Report

BET Surface Area: 10.6561 ± 0.0383 m²/g
Slope: 0.405995 ± 0.001443 g/cm³ STP
Y-Intercept: 0.002523 ± 0.000277 g/cm³ STP
C: 161.941253
Qm: 2.4479 cm³/g STP
Correlation Coefficient: 0.9999432
Molecular Cross-Sectional Area: 0.1620 nm²

Relative Pressure (P/Po)	Quantity Adsorbed (cm³/g STP)	1/[Q(Po/P - 1)]
0.048910454	2.2822	0.022534
0.077386655	2.4522	0.034206
0.095083473	2.5421	0.041333
0.123883388	2.6734	0.052891
0.148628264	2.7840	0.062706
0.173850205	2.8924	0.072755
0.199214129	2.9983	0.082971
0.224543969	3.1044	0.093277
0.250010120	3.2120	0.103784
0.275550098	3.3213	0.114520
0.301305895	3.4329	0.125620

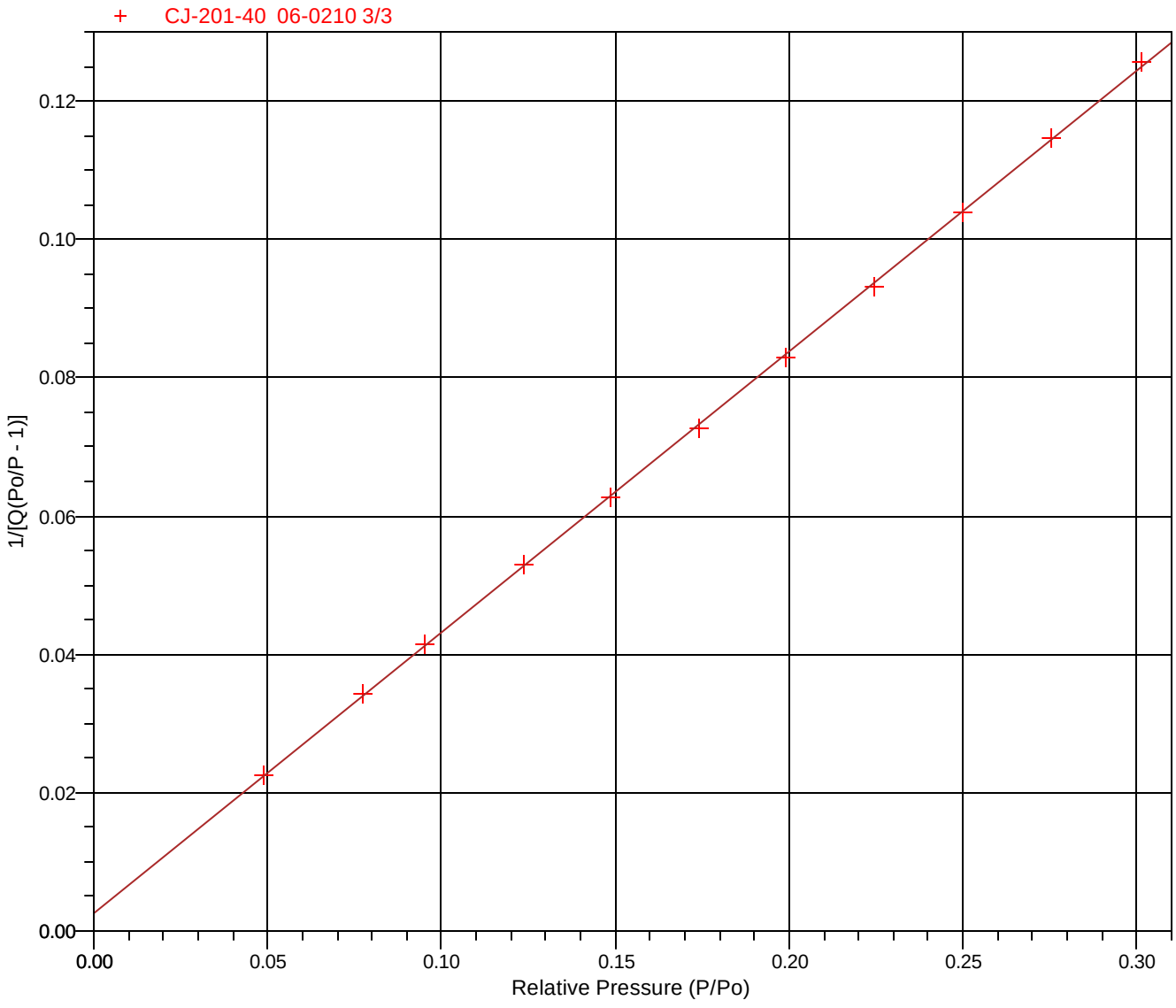
Sample: CJ-201-40 06-0210 3/3
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0210.SMP

Started: 2/1/2006 12:27:55PM
Completed: 2/1/2006 3:23:59PM
Report Time: 2/1/2006 3:24:00PM
Warm Free Space: 5.1716 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.2757 g
Cold Free Space: 14.2717 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Plot



Sample: CJ-201-40 06-0210 3/3
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0210.SMP

Started: 2/1/2006 12:27:55PM
Completed: 2/1/2006 3:23:59PM
Report Time: 2/1/2006 3:24:00PM
Warm Free Space: 5.1716 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.2757 g
Cold Free Space: 14.2717 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Summary Report

Surface Area

Single point surface area at P/Po = 0.301305895: 10.4413 m²/g

BET Surface Area: 10.6561 m²/g

Sample: CJ-202-40 06-0211 38/38
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0211.SMP

Started: 2/1/2006 12:27:55PM
Completed: 2/1/2006 3:23:59PM
Report Time: 2/1/2006 3:42:29PM
Warm Free Space: 6.0917 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.8504 g
Cold Free Space: 17.8637 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Tabular Report

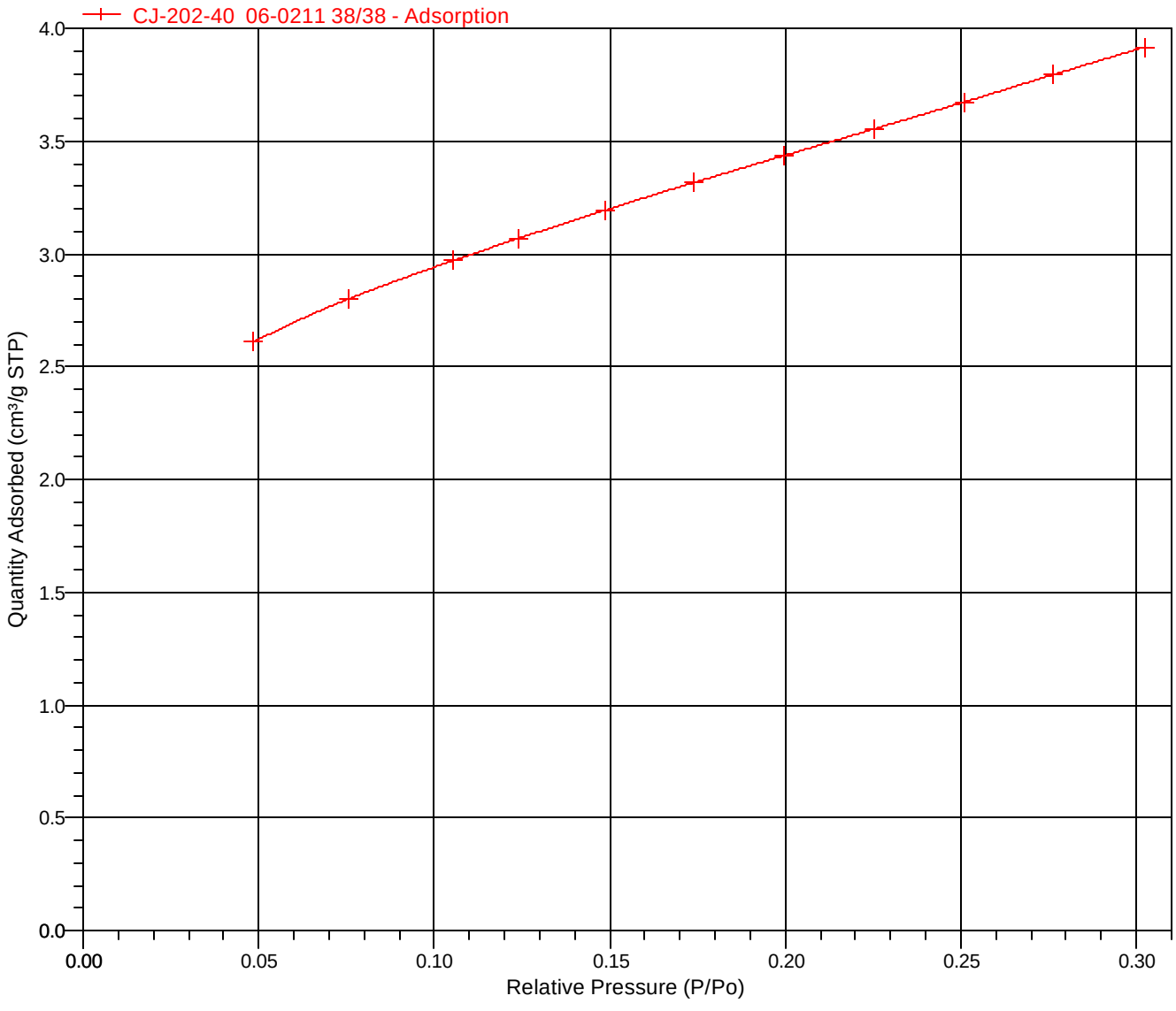
Relative Pressure (P/Po)	Absolute Pressure (mmHg)	Quantity Adsorbed (cm³/g STP)	Elapsed Time (h:min)	Saturation Pressure (mmHg)
			01:10	735.79211
0.048188998	35.45708	2.6084	01:46	
0.075697008	55.69726	2.8007	01:58	
0.105261690	77.45072	2.9694	02:08	
0.124125949	91.33089	3.0685	02:13	
0.148686061	109.40203	3.1933	02:20	
0.174005999	128.03224	3.3160	02:27	
0.199663001	146.91046	3.4353	02:32	
0.225068618	165.60371	3.5540	02:38	
0.250788476	184.52818	3.6731	02:43	
0.276325488	203.31812	3.7943	02:49	
0.302319564	222.44435	3.9175	02:54	

Sample: CJ-202-40 06-0211 38/38
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0211.SMP

Started:	2/1/2006 12:27:55PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 3:23:59PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 3:42:29PM	Sample Mass:	4.8504 g
Warm Free Space:	6.0917 cm³ Measured	Cold Free Space:	17.8637 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Linear Plot



Sample: CJ-202-40 06-0211 38/38
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0211.SMP

Started: 2/1/2006 12:27:55PM
Completed: 2/1/2006 3:23:59PM
Report Time: 2/1/2006 3:42:29PM
Warm Free Space: 6.0917 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.8504 g
Cold Free Space: 17.8637 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Report

BET Surface Area: 12.2117 ± 0.0440 m²/g
Slope: 0.354268 ± 0.001265 g/cm³ STP
Y-Intercept: 0.002211 ± 0.000225 g/cm³ STP
C: 161.265813
Qm: 2.8052 cm³/g STP
Correlation Coefficient: 0.9999490
Molecular Cross-Sectional Area: 0.1620 nm²

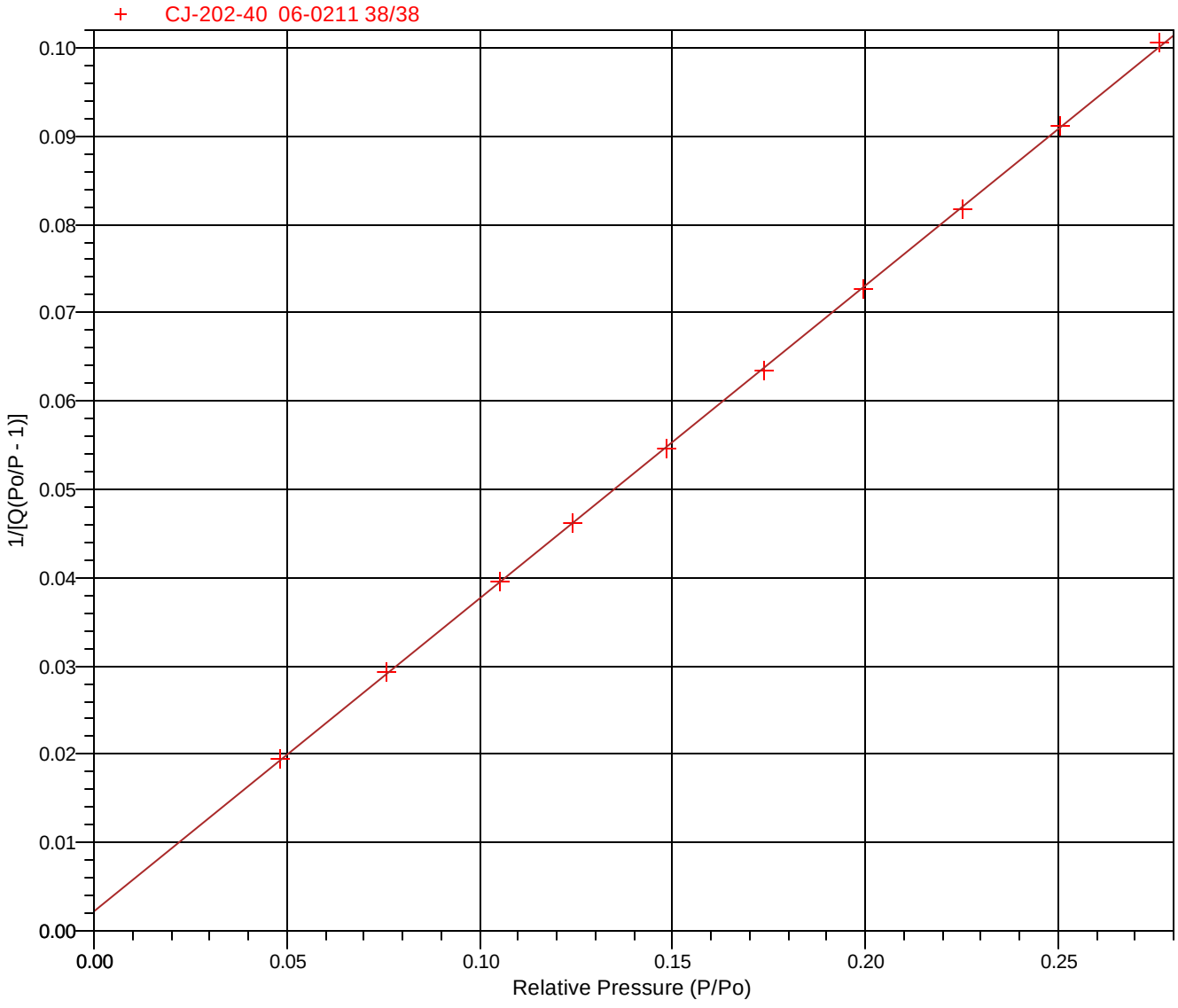
Relative Pressure (P/Po)	Quantity Adsorbed (cm³/g STP)	1/[Q(Po/P - 1)]
0.048188998	2.6084	0.019410
0.075697008	2.8007	0.029241
0.105261690	2.9694	0.039619
0.124125949	3.0685	0.046185
0.148686061	3.1933	0.054694
0.174005999	3.3160	0.063529
0.199663001	3.4353	0.072621
0.225068618	3.5540	0.081722
0.250788476	3.6731	0.091131
0.276325488	3.7943	0.100635

Sample: CJ-202-40 06-0211 38/38
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0211.SMP

Started:	2/1/2006 12:27:55PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 3:23:59PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 3:42:29PM	Sample Mass:	4.8504 g
Warm Free Space:	6.0917 cm³ Measured	Cold Free Space:	17.8637 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Plot



Sample: CJ-202-40 06-0211 38/38
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0211.SMP

Started: 2/1/2006 12:27:55PM
Completed: 2/1/2006 3:23:59PM
Report Time: 2/1/2006 3:42:29PM
Warm Free Space: 6.0917 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.8504 g
Cold Free Space: 17.8637 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Summary Report

Surface Area

Single point surface area at P/Po = 0.276325488: 11.9531 m²/g

BET Surface Area: 12.2117 m²/g

Sample: CJ-203-40 06-0212 815/815
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0212.SMP

Started: 2/1/2006 12:27:55PM
Completed: 2/1/2006 3:23:59PM
Report Time: 2/1/2006 3:24:02PM
Warm Free Space: 5.8383 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.9651 g
Cold Free Space: 16.8406 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Tabular Report

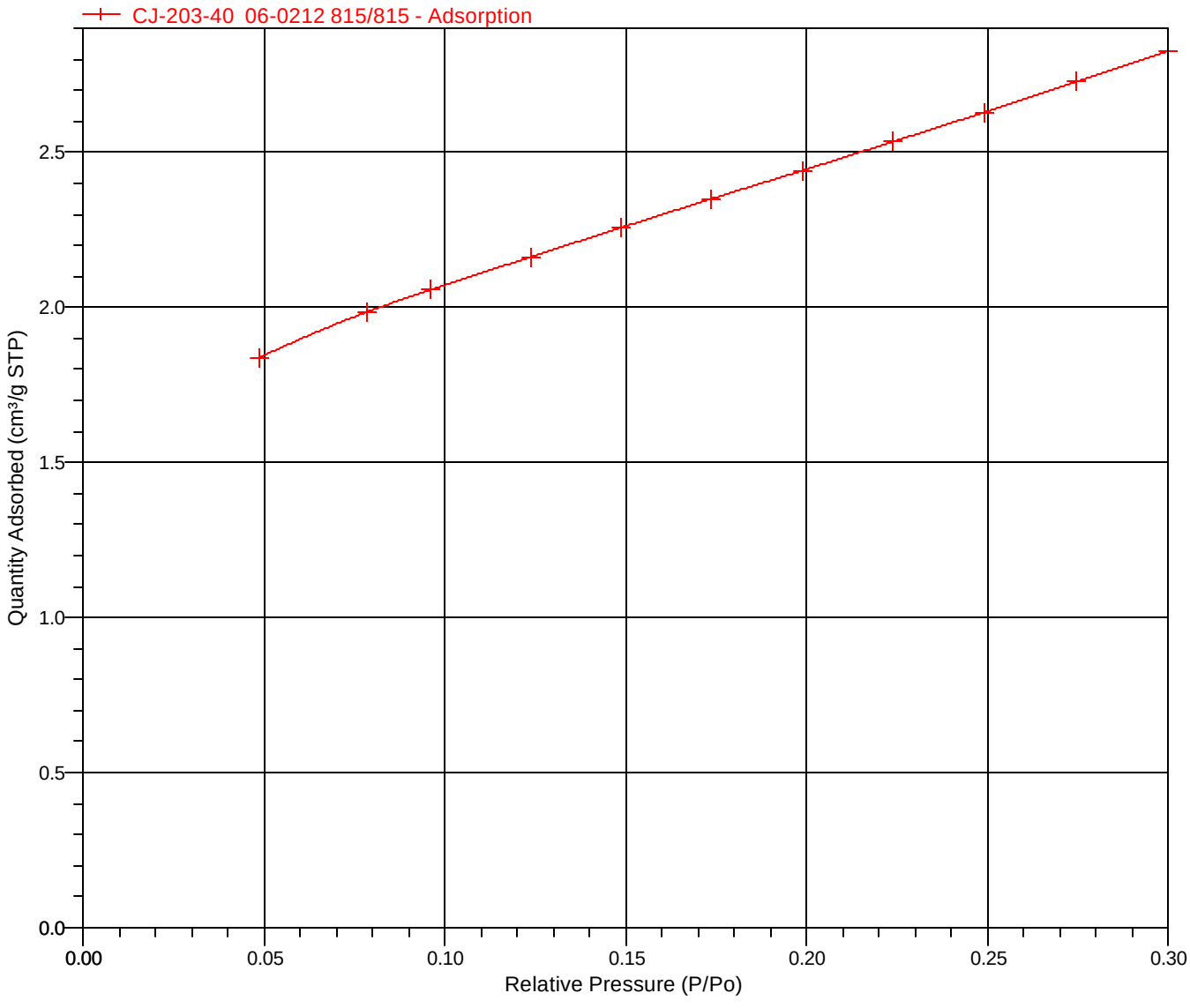
Relative Pressure (P/Po)	Absolute Pressure (mmHg)	Quantity Adsorbed (cm³/g STP)	Elapsed Time (h:min)	Saturation Pressure (mmHg)
			01:10	735.79211
0.048868273	35.95689	1.8390	01:39	
0.078725572	57.92566	1.9854	01:49	
0.095925972	70.58157	2.0561	01:54	
0.123915770	91.17625	2.1632	02:00	
0.148682981	109.39977	2.2569	02:06	
0.173643780	127.76572	2.3496	02:11	
0.198912019	146.35789	2.4415	02:16	
0.224032241	164.84116	2.5341	02:22	
0.249180936	183.34537	2.6292	02:26	
0.274443482	201.93335	2.7267	02:32	
0.299973650	220.71825	2.8268	02:36	

Sample: CJ-203-40 06-0212 815/815
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0212.SMP

Started:	2/1/2006 12:27:55PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 3:23:59PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 3:24:02PM	Sample Mass:	4.9651 g
Warm Free Space:	5.8383 cm³ Measured	Cold Free Space:	16.8406 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Linear Plot



Sample: CJ-203-40 06-0212 815/815
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0212.SMP

Started: 2/1/2006 12:27:55PM
Completed: 2/1/2006 3:23:59PM
Report Time: 2/1/2006 3:24:02PM
Warm Free Space: 5.8383 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.9651 g
Cold Free Space: 16.8406 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Report

BET Surface Area: 8.8087 ± 0.0164 m²/g
Slope: 0.489798 ± 0.000906 g/cm³ STP
Y-Intercept: 0.004396 ± 0.000173 g/cm³ STP
C: 112.409201
Qm: 2.0235 cm³/g STP
Correlation Coefficient: 0.9999846
Molecular Cross-Sectional Area: 0.1620 nm²

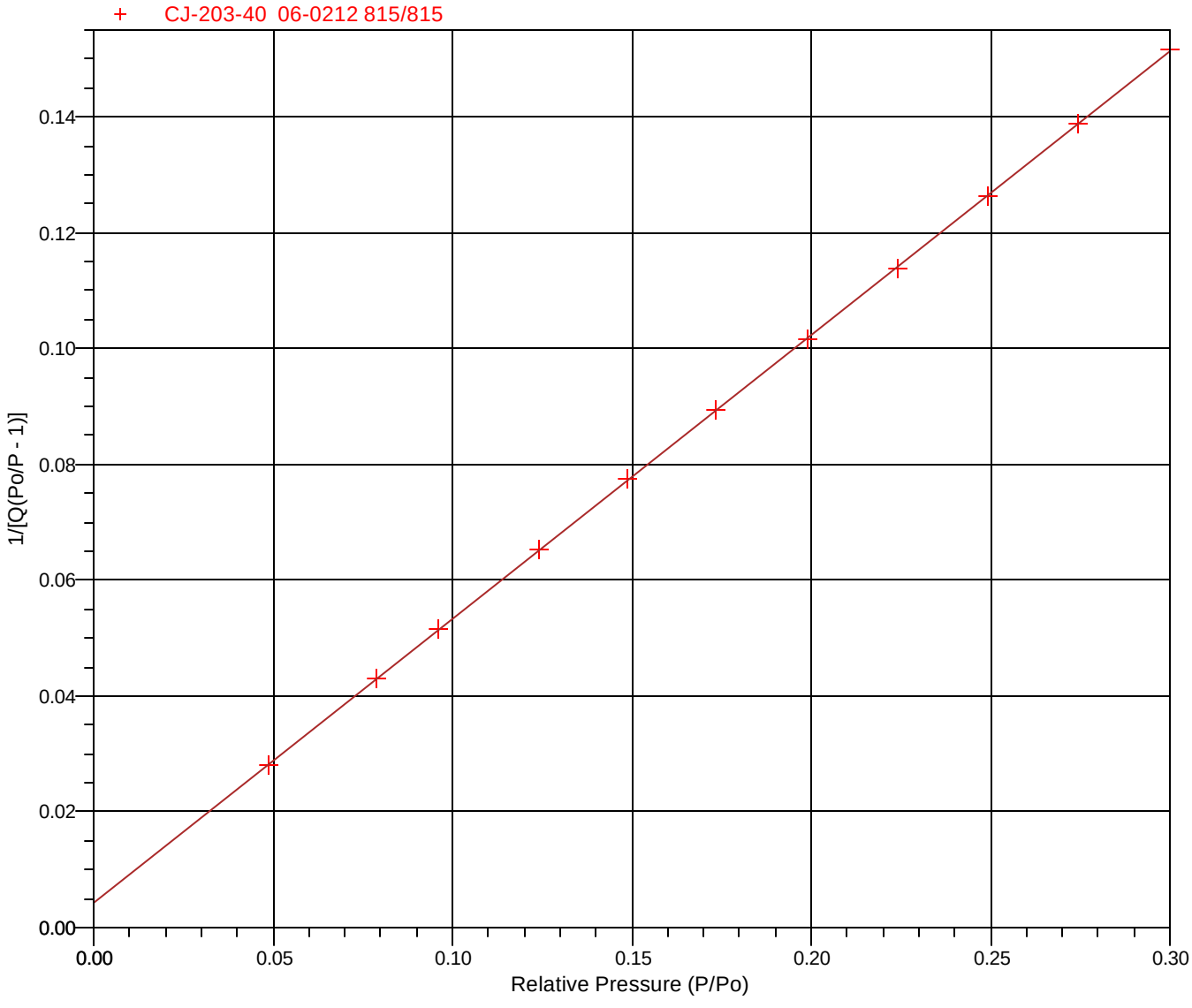
Relative Pressure (P/Po)	Quantity Adsorbed (cm³/g STP)	1/[Q(Po/P - 1)]
0.048868273	1.8390	0.027939
0.078725572	1.9854	0.043041
0.095925972	2.0561	0.051604
0.123915770	2.1632	0.065385
0.148682981	2.2569	0.077385
0.173643780	2.3496	0.089433
0.198912019	2.4415	0.101703
0.224032241	2.5341	0.113929
0.249180936	2.6292	0.126228
0.274443482	2.7267	0.138723
0.299973650	2.8268	0.151593

Sample: CJ-203-40 06-0212 815/815
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0212.SMP

Started:	2/1/2006 12:27:55PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 3:23:59PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 3:24:02PM	Sample Mass:	4.9651 g
Warm Free Space:	5.8383 cm³ Measured	Cold Free Space:	16.8406 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Plot



Sample: CJ-203-40 06-0212 815/815
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0212.SMP

Started:	2/1/2006 12:27:55PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 3:23:59PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 3:24:02PM	Sample Mass:	4.9651 g
Warm Free Space:	5.8383 cm³ Measured	Cold Free Space:	16.8406 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Summary Report

Surface Area

Single point surface area at P/Po = 0.299973650: 8.6142 m²/g

BET Surface Area: 8.8087 m²/g

Sample: CJ-204-40 06-0213 G1/G1
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0213.SMP

Started: 2/1/2006 12:24:05PM
Completed: 2/1/2006 3:16:44PM
Report Time: 2/1/2006 3:43:34PM
Warm Free Space: 5.6492 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.4734 g
Cold Free Space: 16.0508 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Tabular Report

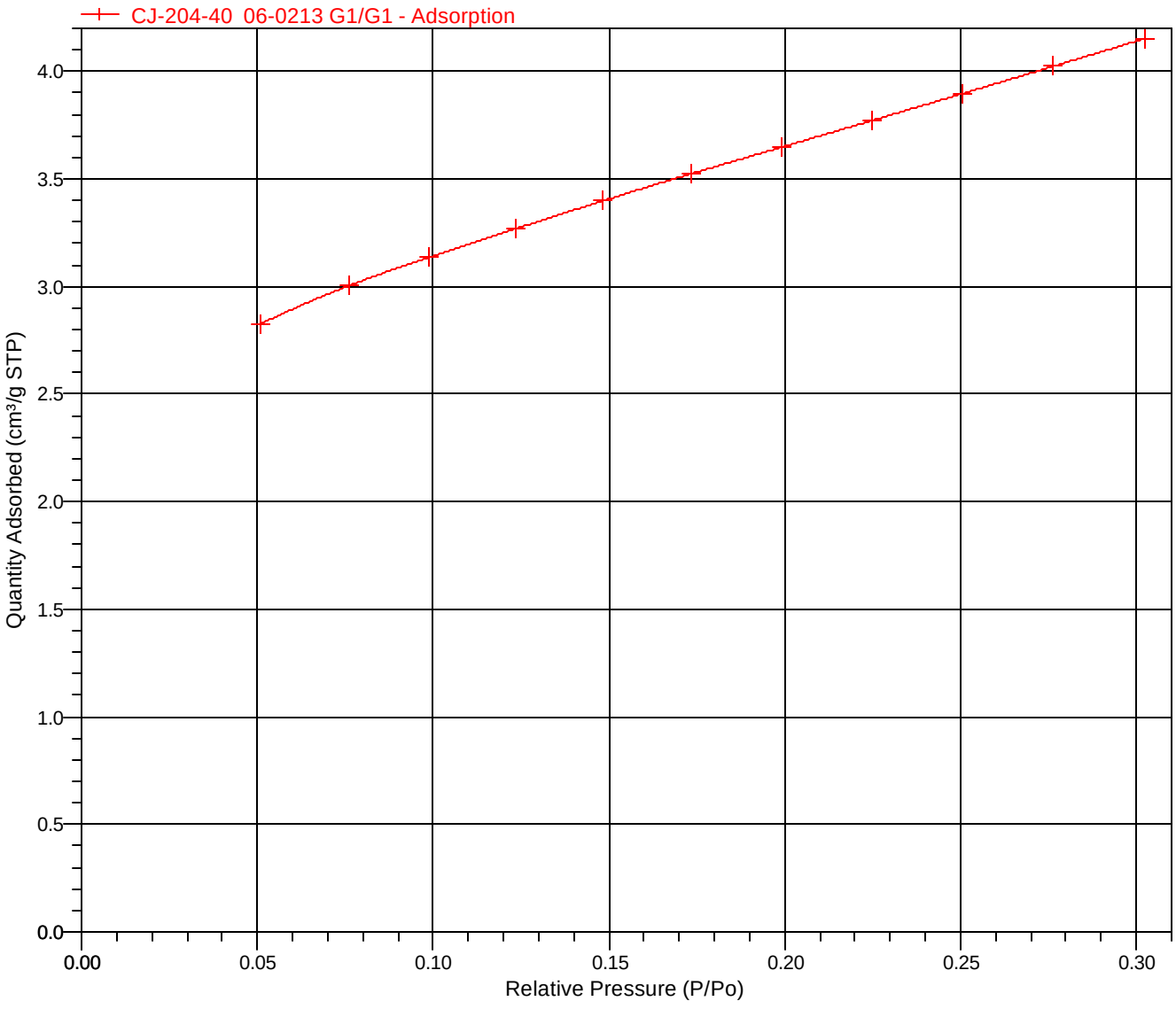
Relative Pressure (P/Po)	Absolute Pressure (mmHg)	Quantity Adsorbed (cm³/g STP)	Elapsed Time (h:min)	Saturation Pressure (mmHg)
			01:13	734.31885
0.051070929	37.50235	2.8265	01:47	
0.076067257	55.85762	3.0041	01:58	
0.098670631	72.45570	3.1361	02:04	
0.123344049	90.57386	3.2685	02:12	
0.148242354	108.85715	3.3977	02:18	
0.173544281	127.43684	3.5242	02:24	
0.199226794	146.29599	3.6479	02:30	
0.224759373	165.04504	3.7714	02:36	
0.250534137	183.97194	3.8965	02:41	
0.276424207	202.98351	4.0230	02:46	
0.302354651	222.02472	4.1525	02:51	

Sample: CJ-204-40 06-0213 G1/G1
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0213.SMP

Started:	2/1/2006 12:24:05PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 3:16:44PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 3:43:34PM	Sample Mass:	4.4734 g
Warm Free Space:	5.6492 cm³ Measured	Cold Free Space:	16.0508 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Linear Plot



Sample: CJ-204-40 06-0213 G1/G1
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0213.SMP

Started: 2/1/2006 12:24:05PM
Completed: 2/1/2006 3:16:44PM
Report Time: 2/1/2006 3:43:34PM
Warm Free Space: 5.6492 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.4734 g
Cold Free Space: 16.0508 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Report

BET Surface Area: 12.9162 ± 0.0501 m²/g
Slope: 0.335315 ± 0.001288 g/cm³ STP
Y-Intercept: 0.001719 ± 0.000229 g/cm³ STP
C: 196.026540
Qm: 2.9671 cm³/g STP
Correlation Coefficient: 0.9999410
Molecular Cross-Sectional Area: 0.1620 nm²

Relative Pressure (P/Po)	Quantity Adsorbed (cm³/g STP)	1/[Q(Po/P - 1)]
0.051070929	2.8265	0.019041
0.076067257	3.0041	0.027406
0.098670631	3.1361	0.034908
0.123344049	3.2685	0.043047
0.148242354	3.3977	0.051223
0.173544281	3.5242	0.059584
0.199226794	3.6479	0.068202
0.224759373	3.7714	0.076873
0.250534137	3.8965	0.085791
0.276424207	4.0230	0.094960

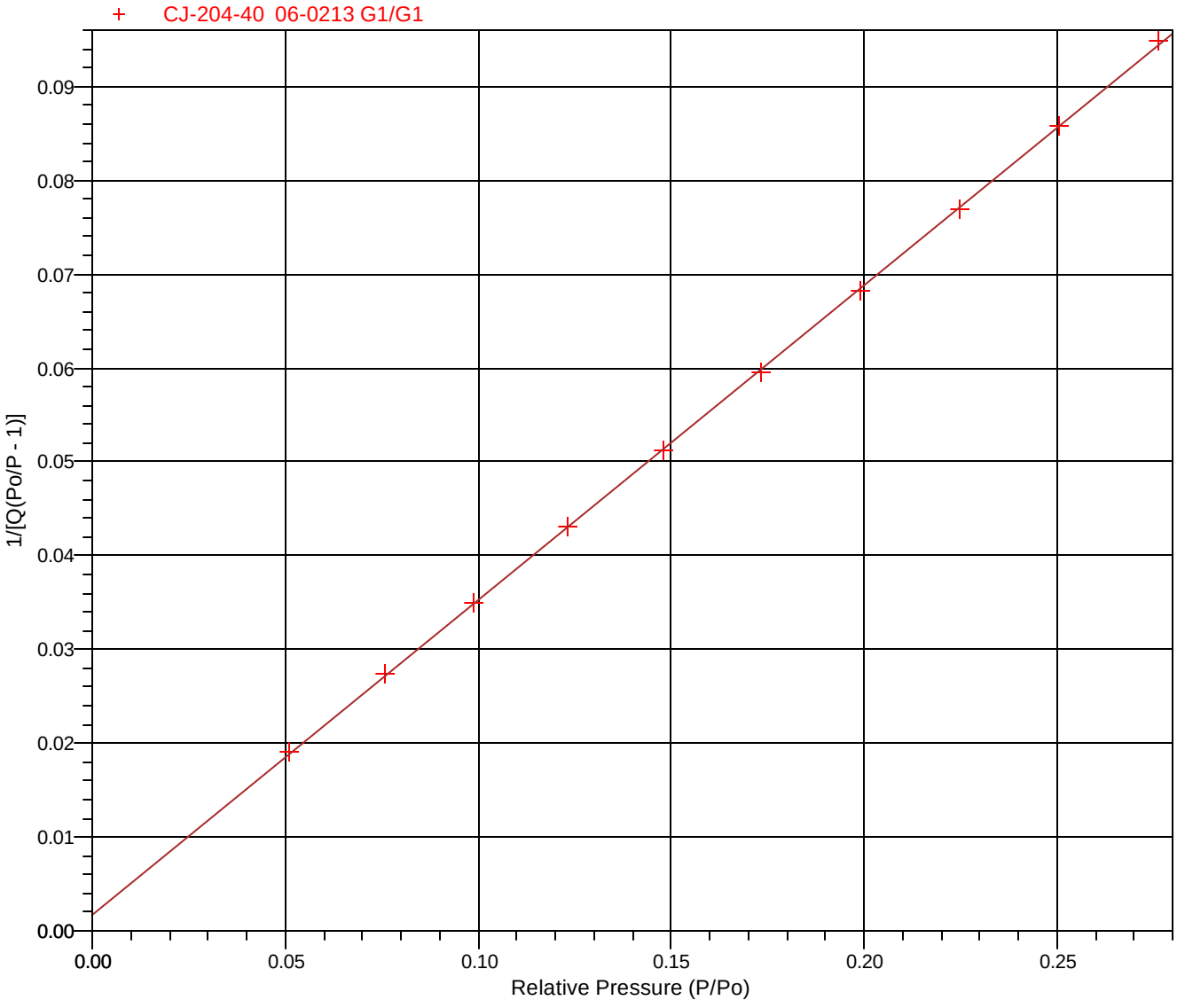
Sample: CJ-204-40 06-0213 G1/G1
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0213.SMP

Started: 2/1/2006 12:24:05PM
Completed: 2/1/2006 3:16:44PM
Report Time: 2/1/2006 3:43:34PM
Warm Free Space: 5.6492 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.4734 g
Cold Free Space: 16.0508 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Plot



Sample: CJ-204-40 06-0213 G1/G1
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0213.SMP

Started: 2/1/2006 12:24:05PM
Completed: 2/1/2006 3:16:44PM
Report Time: 2/1/2006 3:43:34PM
Warm Free Space: 5.6492 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.4734 g
Cold Free Space: 16.0508 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Summary Report

Surface Area

Single point surface area at P/Po = 0.276424207: 12.6720 m²/g

BET Surface Area: 12.9162 m²/g

Sample: CJ-205-40 06-0214 G2/G2
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0214.SMP

Started: 2/1/2006 12:24:05PM
Completed: 2/1/2006 3:16:44PM
Report Time: 2/1/2006 3:16:49PM
Warm Free Space: 5.6027 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.2657 g
Cold Free Space: 15.9013 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Tabular Report

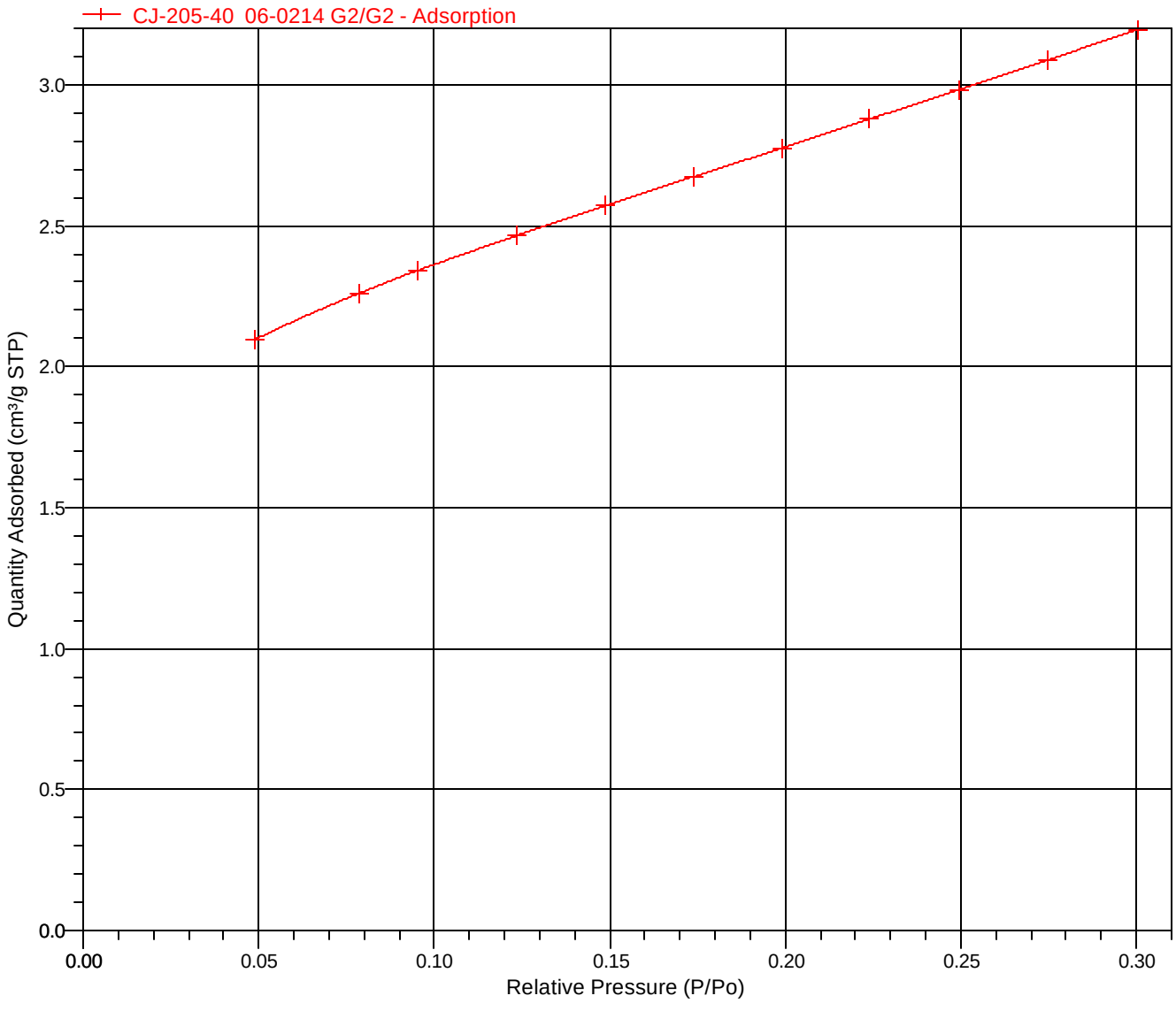
Relative Pressure (P/Po)	Absolute Pressure (mmHg)	Quantity Adsorbed (cm³/g STP)	Elapsed Time (h:min)	Saturation Pressure (mmHg)
			01:13	734.31885
0.049028719	36.00271	2.0965	01:39	
0.078428859	57.59179	2.2602	01:46	
0.095402314	70.05572	2.3412	01:53	
0.123514763	90.69922	2.4647	02:01	
0.148487792	109.03738	2.5710	02:06	
0.173677332	127.53454	2.6739	02:11	
0.198861179	146.02751	2.7753	02:16	
0.224033607	164.51210	2.8776	02:21	
0.249320011	183.08038	2.9817	02:26	
0.274777348	201.77419	3.0875	02:31	
0.300337231	220.54329	3.1959	02:36	

Sample: CJ-205-40 06-0214 G2/G2
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0214.SMP

Started:	2/1/2006 12:24:05PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 3:16:44PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 3:16:49PM	Sample Mass:	4.2657 g
Warm Free Space:	5.6027 cm³ Measured	Cold Free Space:	15.9013 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Linear Plot



Sample: CJ-205-40 06-0214 G2/G2
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0214.SMP

Started: 2/1/2006 12:24:05PM
Completed: 2/1/2006 3:16:44PM
Report Time: 2/1/2006 3:16:49PM
Warm Free Space: 5.6027 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.2657 g
Cold Free Space: 15.9013 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Report

BET Surface Area: 9.9511 ± 0.0246 m²/g
Slope: 0.434049 ± 0.001061 g/cm³ STP
Y-Intercept: 0.003410 ± 0.000203 g/cm³ STP
C: 128.300420
Qm: 2.2859 cm³/g STP
Correlation Coefficient: 0.9999731
Molecular Cross-Sectional Area: 0.1620 nm²

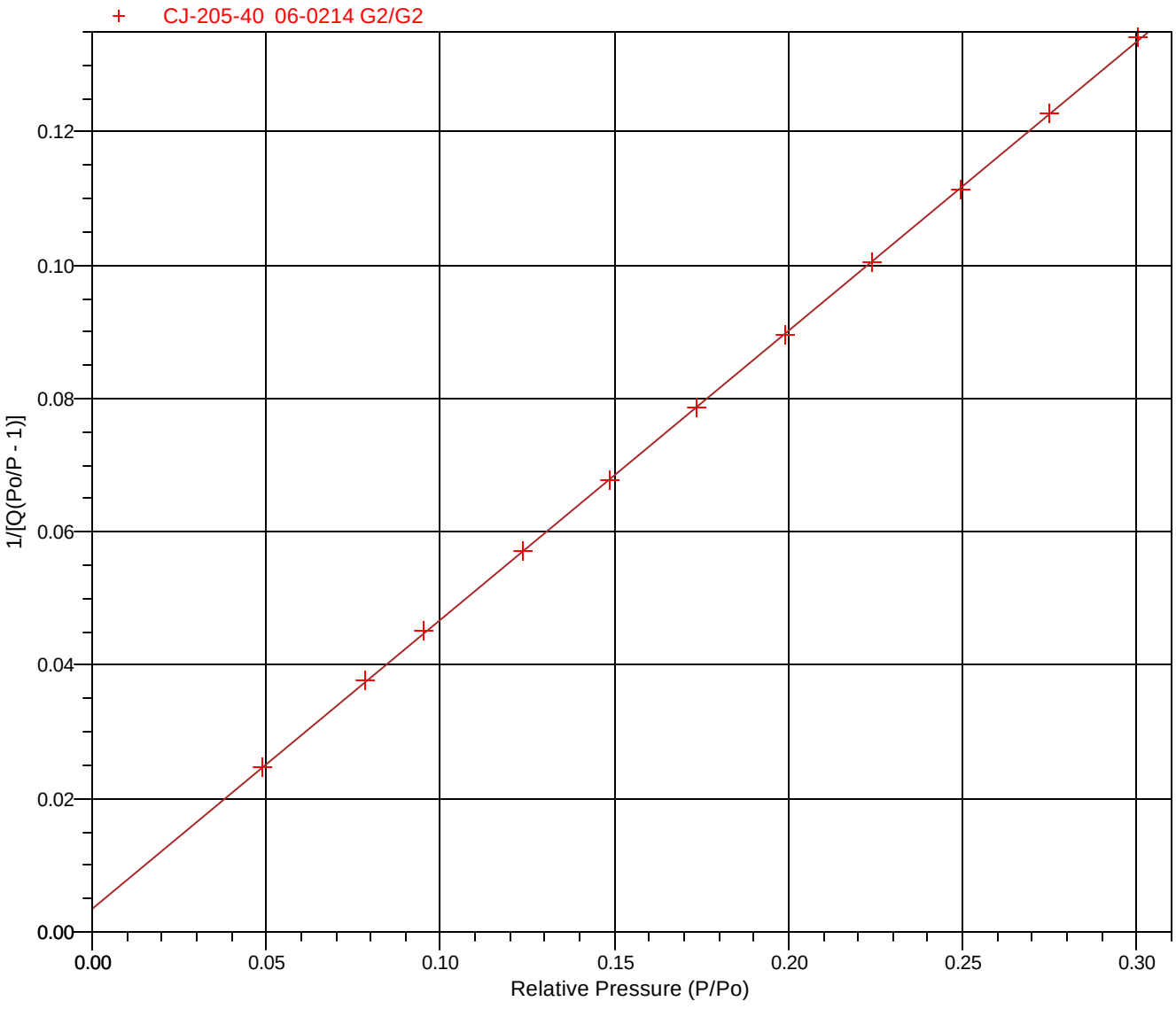
Relative Pressure (P/Po)	Quantity Adsorbed (cm³/g STP)	1/[Q(Po/P - 1)]
0.049028719	2.0965	0.024591
0.078428859	2.2602	0.037652
0.095402314	2.3412	0.045048
0.123514763	2.4647	0.057175
0.148487792	2.5710	0.067826
0.173677332	2.6739	0.078604
0.198861179	2.7753	0.089441
0.224033607	2.8776	0.100333
0.249320011	2.9817	0.111387
0.274777348	3.0875	0.122716
0.300337231	3.1959	0.134314

Sample: CJ-205-40 06-0214 G2/G2
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0214.SMP

Started:	2/1/2006 12:24:05PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 3:16:44PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 3:16:49PM	Sample Mass:	4.2657 g
Warm Free Space:	5.6027 cm³ Measured	Cold Free Space:	15.9013 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Plot



Sample: CJ-205-40 06-0214 G2/G2
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0214.SMP

Started:	2/1/2006 12:24:05PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 3:16:44PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 3:16:49PM	Sample Mass:	4.2657 g
Warm Free Space:	5.6027 cm³ Measured	Cold Free Space:	15.9013 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Summary Report

Surface Area

Single point surface area at P/Po = 0.300337231: 9.7341 m²/g

BET Surface Area: 9.9511 m²/g

Sample: CJ-210-40 06-0220 N6/N6
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0220.SMP

Started: 2/1/2006 4:23:29PM
Completed: 2/1/2006 7:40:08PM
Report Time: 2/2/2006 7:51:21AM
Warm Free Space: 5.6495 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 5.1428 g
Cold Free Space: 16.1759 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Tabular Report

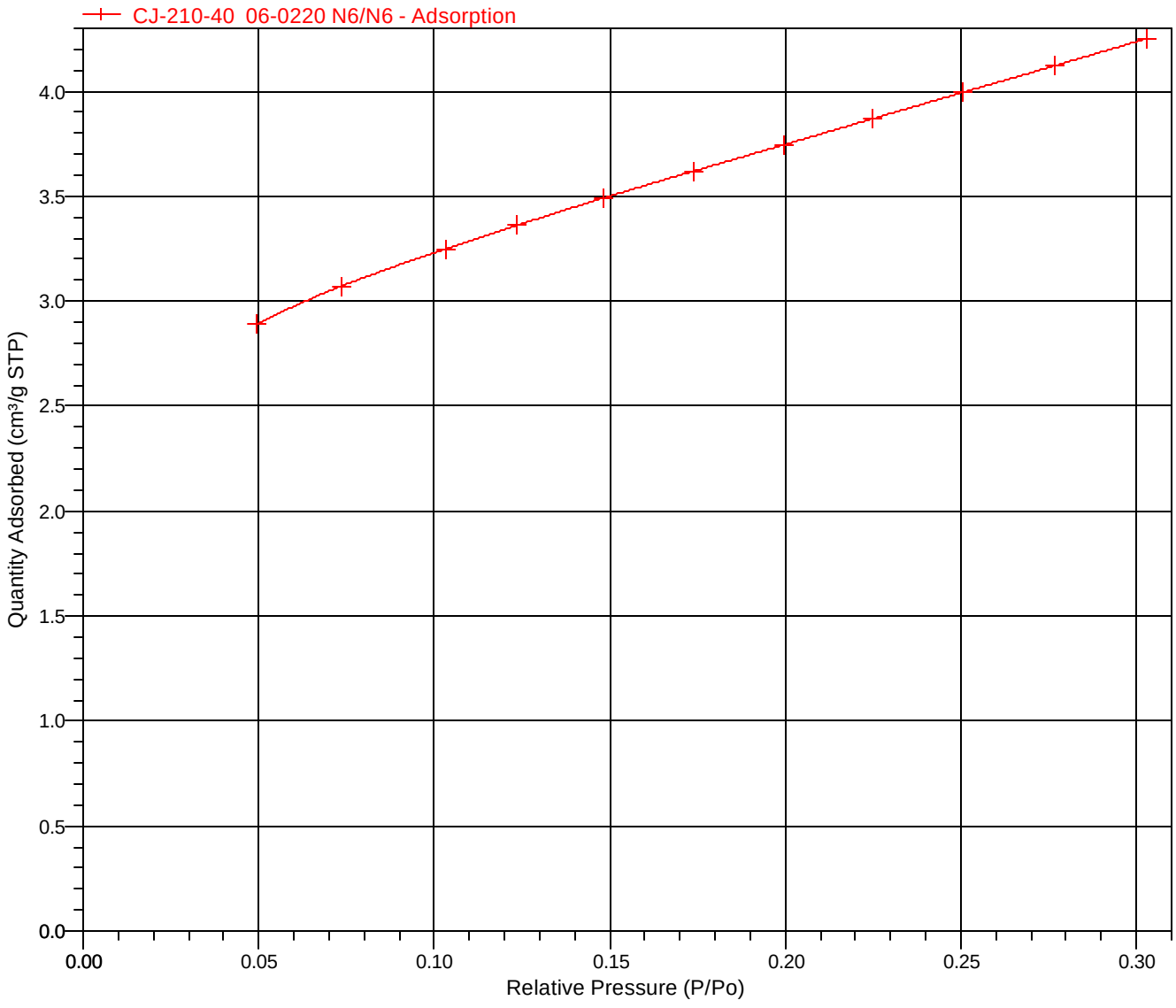
Relative Pressure (P/Po)	Absolute Pressure (mmHg)	Quantity Adsorbed (cm³/g STP)	Elapsed Time (h:min)	Saturation Pressure (mmHg)
			01:10	736.09106
0.049305304	36.29458	2.8912	01:51	
0.073760837	54.29753	3.0722	02:06	
0.103302563	76.04499	3.2499	02:19	
0.123540210	90.94355	3.3609	02:29	
0.148244880	109.13059	3.4916	02:37	
0.173779264	127.92847	3.6198	02:43	
0.199364321	146.76399	3.7447	02:50	
0.224954724	165.60370	3.8690	02:57	
0.250692811	184.55220	3.9948	03:03	
0.276623808	203.64293	4.1218	03:09	
			03:11	736.17419
0.302748904	222.87593	4.2511	03:15	

Sample: CJ-210-40 06-0220 N6/N6
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0220.SMP

Started:	2/1/2006 4:23:29PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 7:40:08PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/2/2006 7:51:21AM	Sample Mass:	5.1428 g
Warm Free Space:	5.6495 cm³ Measured	Cold Free Space:	16.1759 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Linear Plot



Sample: CJ-210-40 06-0220 N6/N6
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0220.SMP

Started: 2/1/2006 4:23:29PM
Completed: 2/1/2006 7:40:08PM
Report Time: 2/2/2006 7:51:21AM
Warm Free Space: 5.6495 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 5.1428 g
Cold Free Space: 16.1759 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Report

BET Surface Area: 13.2247 ± 0.0591 m²/g
Slope: 0.327644 ± 0.001449 g/cm³ STP
Y-Intercept: 0.001529 ± 0.000258 g/cm³ STP
C: 215.310851
Qm: 3.0379 cm³/g STP
Correlation Coefficient: 0.9999217
Molecular Cross-Sectional Area: 0.1620 nm²

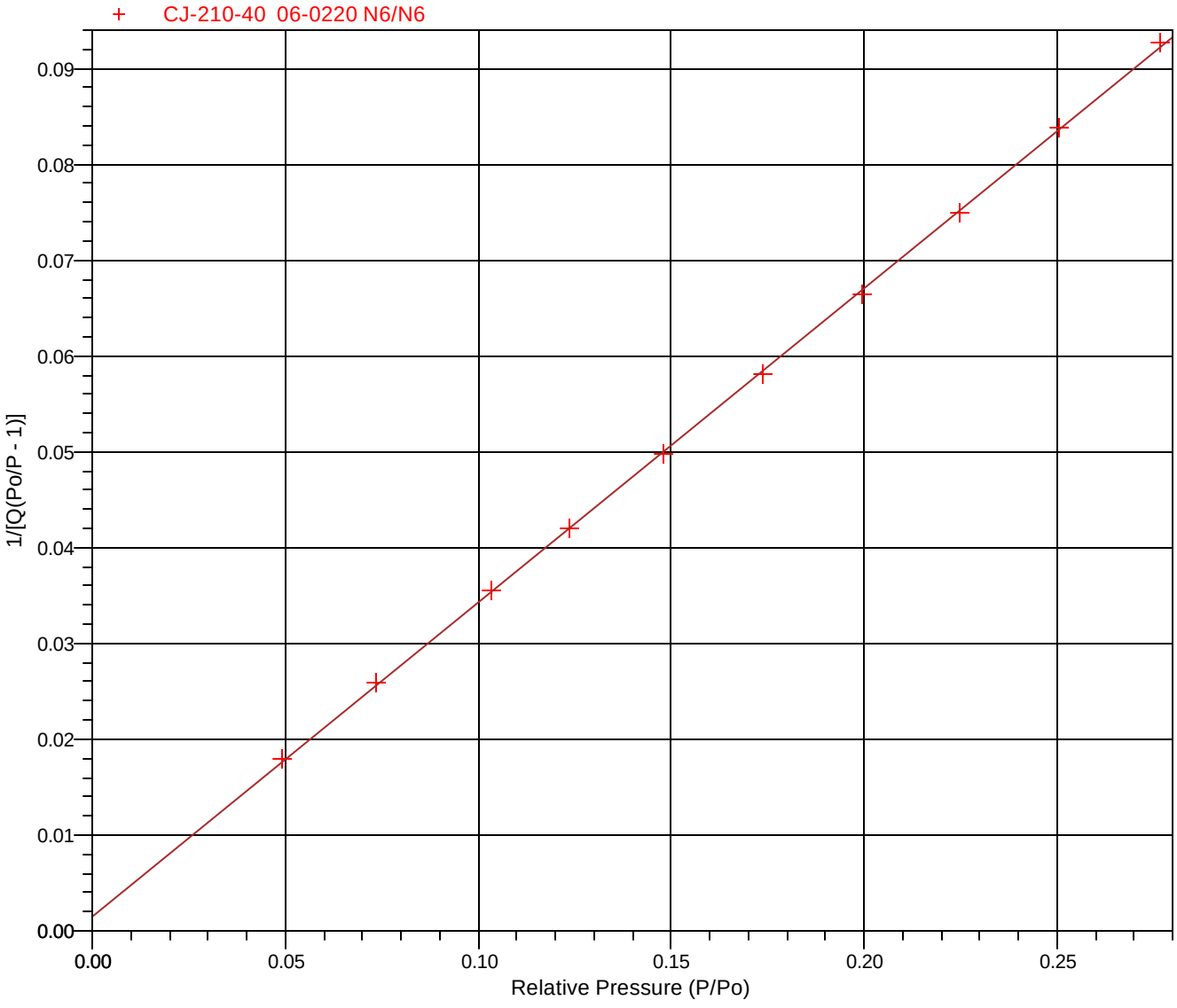
Relative Pressure (P/Po)	Quantity Adsorbed (cm³/g STP)	1/[Q(Po/P - 1)]
0.049305304	2.8912	0.017938
0.073760837	3.0722	0.025921
0.103302563	3.2499	0.035448
0.123540210	3.3609	0.041939
0.148244880	3.4916	0.049847
0.173779264	3.6198	0.058106
0.199364321	3.7447	0.066495
0.224954724	3.8690	0.075018
0.250692811	3.9948	0.083751
0.276623808	4.1218	0.092777

Sample: CJ-210-40 06-0220 N6/N6
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0220.SMP

Started:	2/1/2006 4:23:29PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 7:40:08PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/2/2006 7:51:21AM	Sample Mass:	5.1428 g
Warm Free Space:	5.6495 cm³ Measured	Cold Free Space:	16.1759 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Plot



Sample: CJ-210-40 06-0220 N6/N6
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0220.SMP

Started: 2/1/2006 4:23:29PM
Completed: 2/1/2006 7:40:08PM
Report Time: 2/2/2006 7:51:21AM
Warm Free Space: 5.6495 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 5.1428 g
Cold Free Space: 16.1759 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Summary Report

Surface Area

Single point surface area at P/Po = 0.276623808: 12.9795 m²/g

BET Surface Area: 13.2247 m²/g

Sample: CJ-209-40 06-0219 N5/N5
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0219.SMP

Started: 2/1/2006 4:23:29PM
Completed: 2/1/2006 7:40:08PM
Report Time: 2/1/2006 7:40:06PM
Warm Free Space: 5.4357 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 5.1155 g
Cold Free Space: 15.2828 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Tabular Report

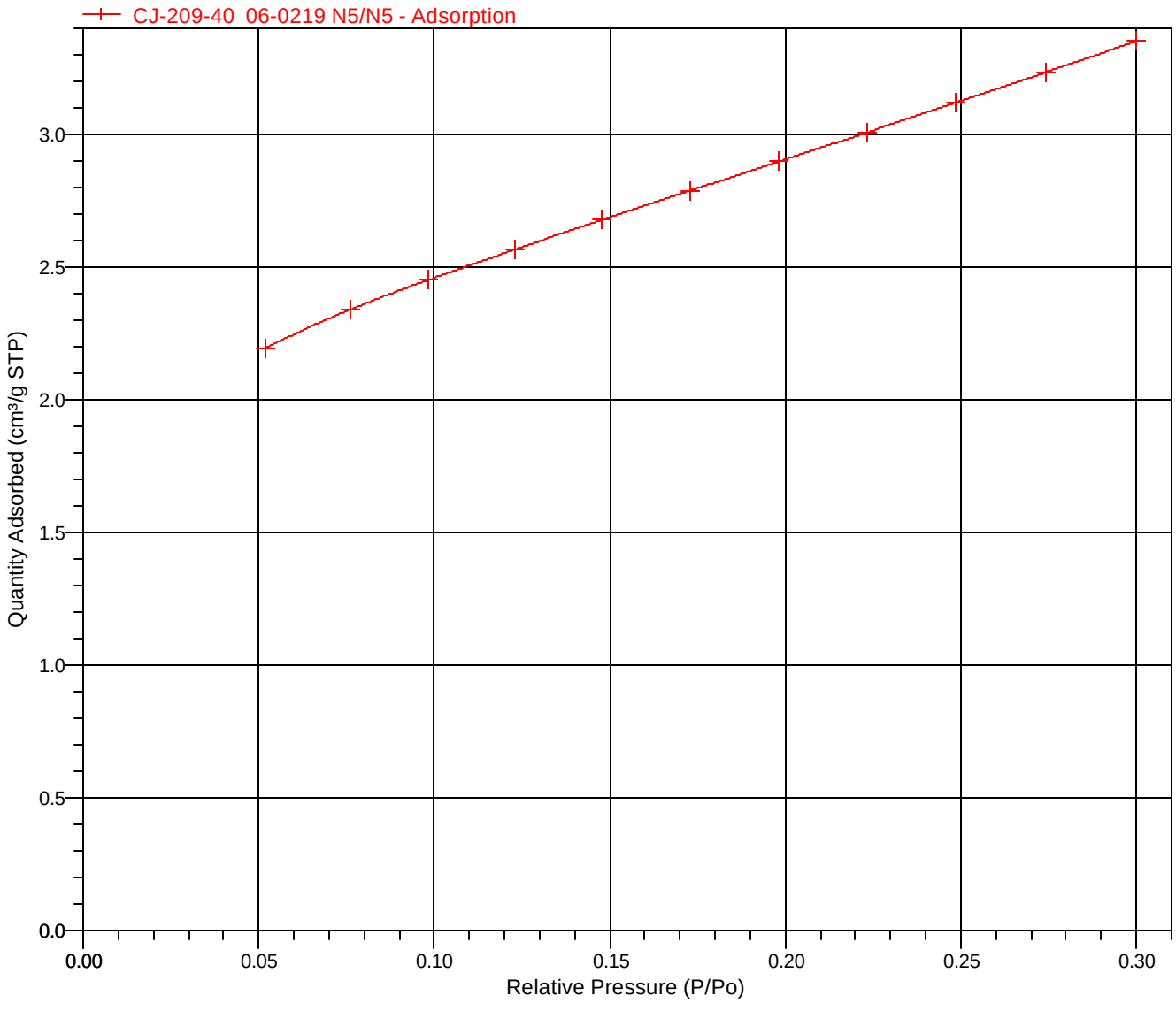
Relative Pressure (P/Po)	Absolute Pressure (mmHg)	Quantity Adsorbed (cm³/g STP)	Elapsed Time (h:min)	Saturation Pressure (mmHg)
			01:10	736.09106
0.051788686	38.12119	2.1947	01:36	
0.076204501	56.09345	2.3405	01:47	
0.098370893	72.40993	2.4519	01:55	
0.122832732	90.41608	2.5662	02:03	
0.147622492	108.66360	2.6782	02:09	
0.172751686	127.16097	2.7882	02:15	
0.197898138	145.67105	2.8976	02:21	
0.223314975	164.38016	3.0077	02:27	
0.248559218	182.96222	3.1200	02:32	
0.274240708	201.86613	3.2344	02:37	
0.300100534	220.90132	3.3510	02:42	

Sample: CJ-209-40 06-0219 N5/N5
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0219.SMP

Started:	2/1/2006 4:23:29PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 7:40:08PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 7:40:06PM	Sample Mass:	5.1155 g
Warm Free Space:	5.4357 cm³ Measured	Cold Free Space:	15.2828 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Linear Plot



Sample: CJ-209-40 06-0219 N5/N5
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0219.SMP

Started: 2/1/2006 4:23:29PM
Completed: 2/1/2006 7:40:08PM
Report Time: 2/1/2006 7:40:06PM
Warm Free Space: 5.4357 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 5.1155 g
Cold Free Space: 15.2828 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Report

BET Surface Area: 10.4560 ± 0.0226 m²/g
Slope: 0.412643 ± 0.000883 g/cm³ STP
Y-Intercept: 0.003694 ± 0.000169 g/cm³ STP
C: 112.707884
Qm: 2.4019 cm³/g STP
Correlation Coefficient: 0.9999794
Molecular Cross-Sectional Area: 0.1620 nm²

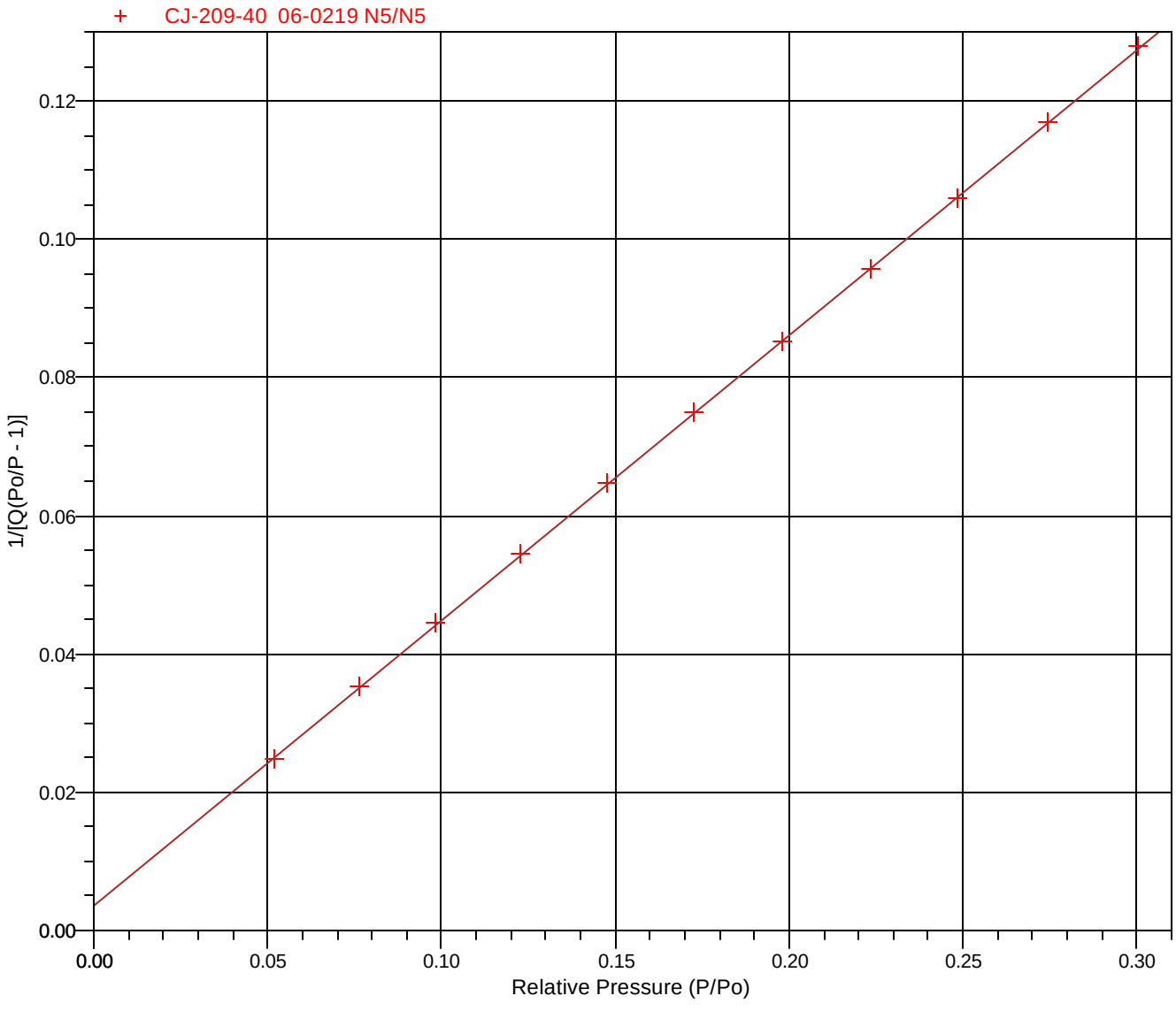
Relative Pressure (P/Po)	Quantity Adsorbed (cm³/g STP)	1/[Q(Po/P - 1)]
0.051788686	2.1947	0.024886
0.076204501	2.3405	0.035244
0.098370893	2.4519	0.044498
0.122832732	2.5662	0.054568
0.147622492	2.6782	0.064665
0.172751686	2.7882	0.074897
0.197898138	2.8976	0.085148
0.223314975	3.0077	0.095596
0.248559218	3.1200	0.106018
0.274240708	3.2344	0.116828
0.300100534	3.3510	0.127954

Sample: CJ-209-40 06-0219 N5/N5
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0219.SMP

Started:	2/1/2006 4:23:29PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 7:40:08PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 7:40:06PM	Sample Mass:	5.1155 g
Warm Free Space:	5.4357 cm³ Measured	Cold Free Space:	15.2828 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Plot



Sample: CJ-209-40 06-0219 N5/N5
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0219.SMP

Started: 2/1/2006 4:23:29PM
Completed: 2/1/2006 7:40:08PM
Report Time: 2/1/2006 7:40:06PM
Warm Free Space: 5.4357 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 5.1155 g
Cold Free Space: 15.2828 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Summary Report

Surface Area

Single point surface area at P/Po = 0.300100534: 10.2099 m²/g

BET Surface Area: 10.4560 m²/g

Sample: CJ-208-40 06-0218 N2/N2
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0218.SMP

Started: 2/1/2006 4:22:41PM
Completed: 2/1/2006 8:12:53PM
Report Time: 2/1/2006 8:12:55PM
Warm Free Space: 5.7202 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.3662 g
Cold Free Space: 16.4086 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Tabular Report

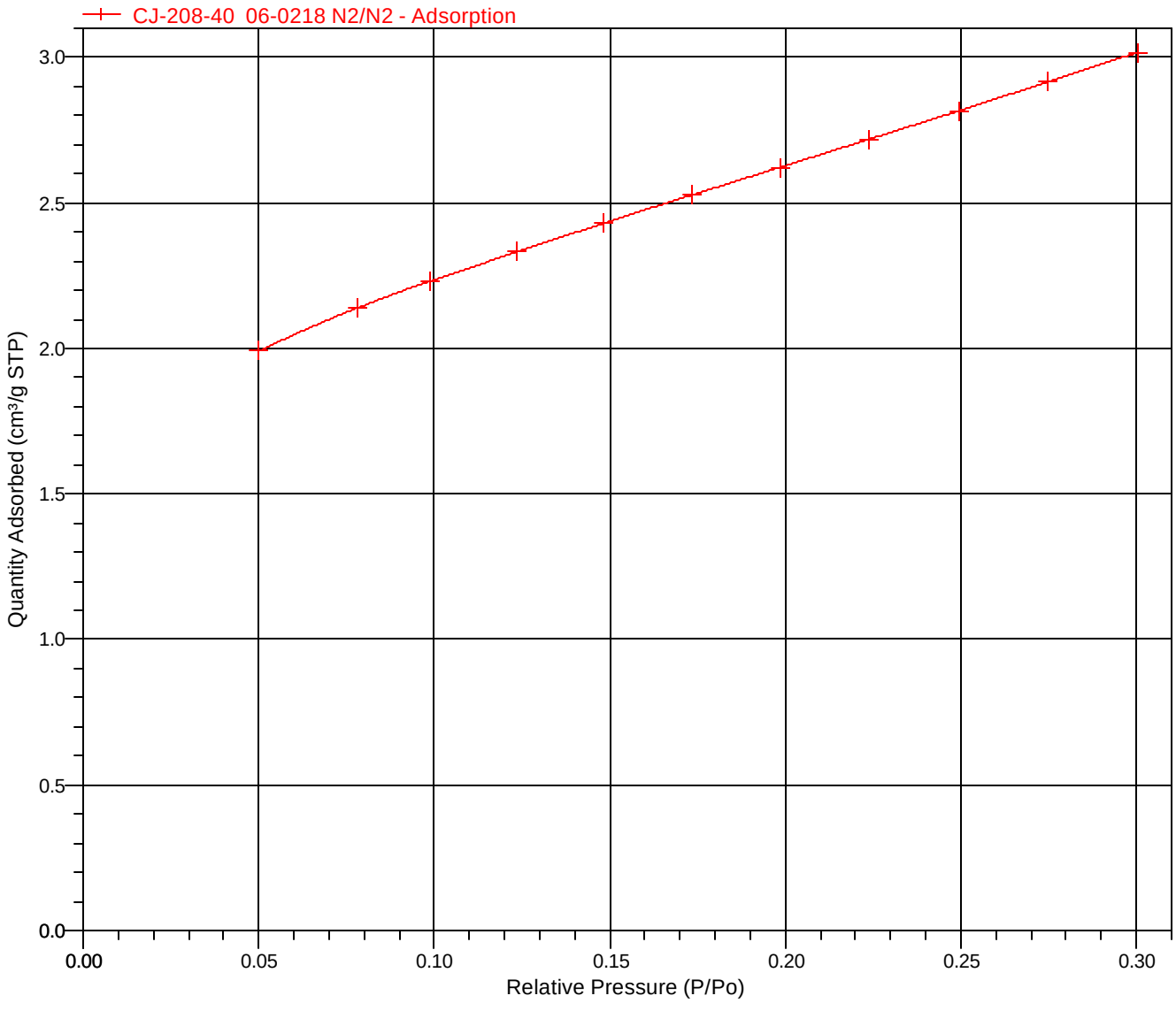
Relative Pressure (P/Po)	Absolute Pressure (mmHg)	Quantity Adsorbed (cm³/g STP)	Elapsed Time (h:min)	Saturation Pressure (mmHg)
			01:08	736.94562
0.050132413	36.94486	1.9911	01:38	
0.078159955	57.59964	2.1391	01:47	
0.098735843	72.76295	2.2310	01:57	
0.123546271	91.04688	2.3313	02:03	
0.148265749	109.26379	2.4301	02:08	
0.173383114	127.77393	2.5273	02:13	
0.198727824	146.45160	2.6228	02:18	
0.224004352	165.07903	2.7188	02:24	
0.249400225	183.79440	2.8166	02:28	
0.274898405	202.58517	2.9161	02:33	
0.300589849	221.51837	3.0177	02:38	

Sample: CJ-208-40 06-0218 N2/N2
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0218.SMP

Started:	2/1/2006 4:22:41PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 8:12:53PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 8:12:55PM	Sample Mass:	4.3662 g
Warm Free Space:	5.7202 cm³ Measured	Cold Free Space:	16.4086 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Linear Plot



Sample: CJ-208-40 06-0218 N2/N2
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0218.SMP

Started: 2/1/2006 4:22:41PM
Completed: 2/1/2006 8:12:53PM
Report Time: 2/1/2006 8:12:55PM
Warm Free Space: 5.7202 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.3662 g
Cold Free Space: 16.4086 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Report

BET Surface Area: 9.3897 ± 0.0250 m²/g
Slope: 0.460156 ± 0.001212 g/cm³ STP
Y-Intercept: 0.003458 ± 0.000232 g/cm³ STP
C: 134.056409
Qm: 2.1570 cm³/g STP
Correlation Coefficient: 0.9999688
Molecular Cross-Sectional Area: 0.1620 nm²

Relative Pressure (P/Po)	Quantity Adsorbed (cm³/g STP)	1/[Q(Po/P - 1)]
0.050132413	1.9911	0.026507
0.078159955	2.1391	0.039637
0.098735843	2.2310	0.049105
0.123546271	2.3313	0.060466
0.148265749	2.4301	0.071634
0.173383114	2.5273	0.082995
0.198727824	2.6228	0.094562
0.224004352	2.7188	0.106174
0.249400225	2.8166	0.117966
0.274898405	2.9161	0.130006
0.300589849	3.0177	0.142417

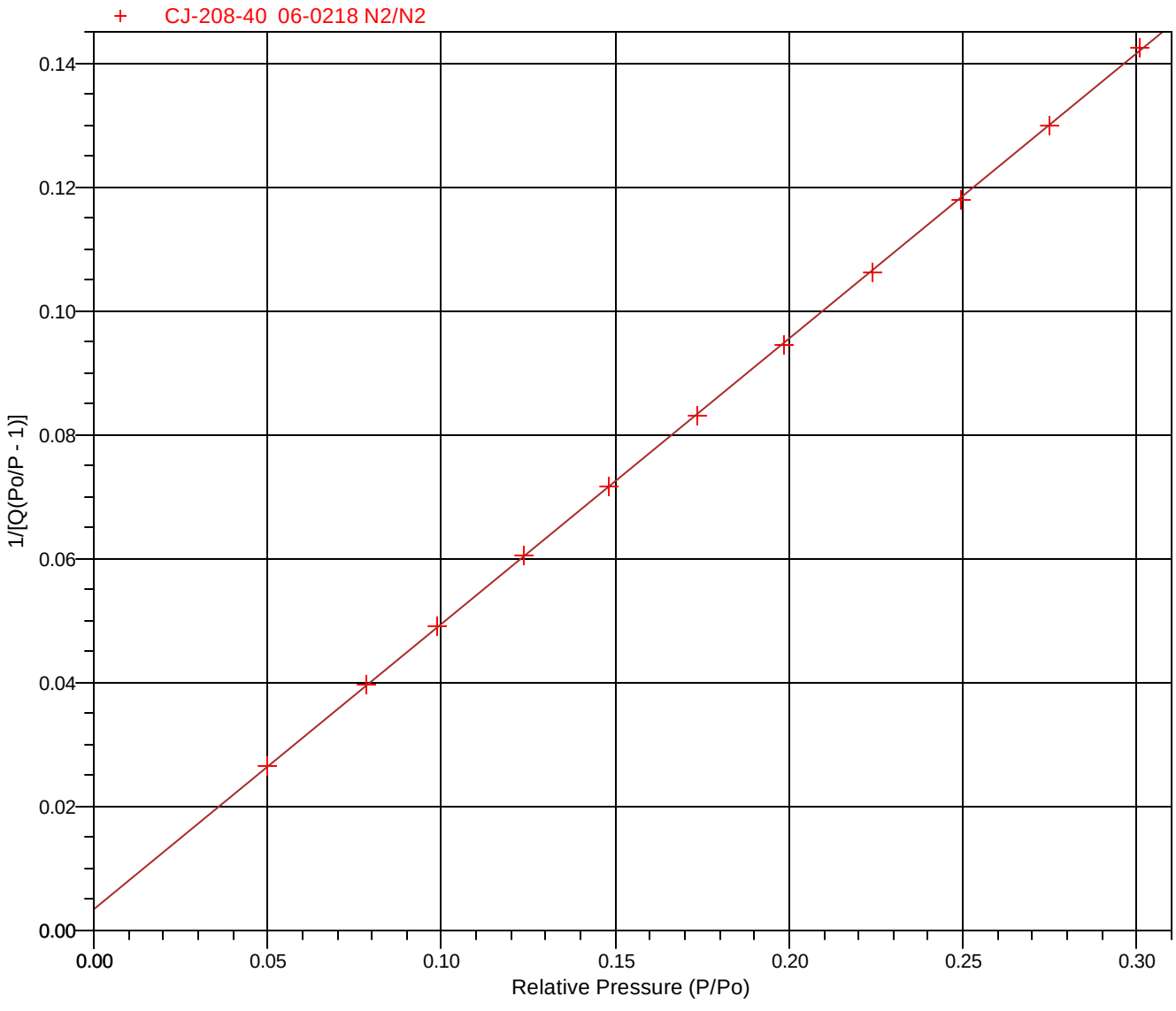
Sample: CJ-208-40 06-0218 N2/N2
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0218.SMP

Started: 2/1/2006 4:22:41PM
Completed: 2/1/2006 8:12:53PM
Report Time: 2/1/2006 8:12:55PM
Warm Free Space: 5.7202 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.3662 g
Cold Free Space: 16.4086 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Plot



Sample: CJ-208-40 06-0218 N2/N2
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0218.SMP

Started:	2/1/2006 4:22:41PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 8:12:53PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 8:12:55PM	Sample Mass:	4.3662 g
Warm Free Space:	5.7202 cm³ Measured	Cold Free Space:	16.4086 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Summary Report

Surface Area

Single point surface area at P/Po = 0.300589849: 9.1880 m²/g

BET Surface Area: 9.3897 m²/g

Sample: CJ-207-40 06-0217 N1/N1
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0217.SMP

Started: 2/1/2006 4:22:41PM
Completed: 2/1/2006 8:12:53PM
Report Time: 2/2/2006 7:50:36AM
Warm Free Space: 5.5902 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.3543 g
Cold Free Space: 15.9894 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Tabular Report

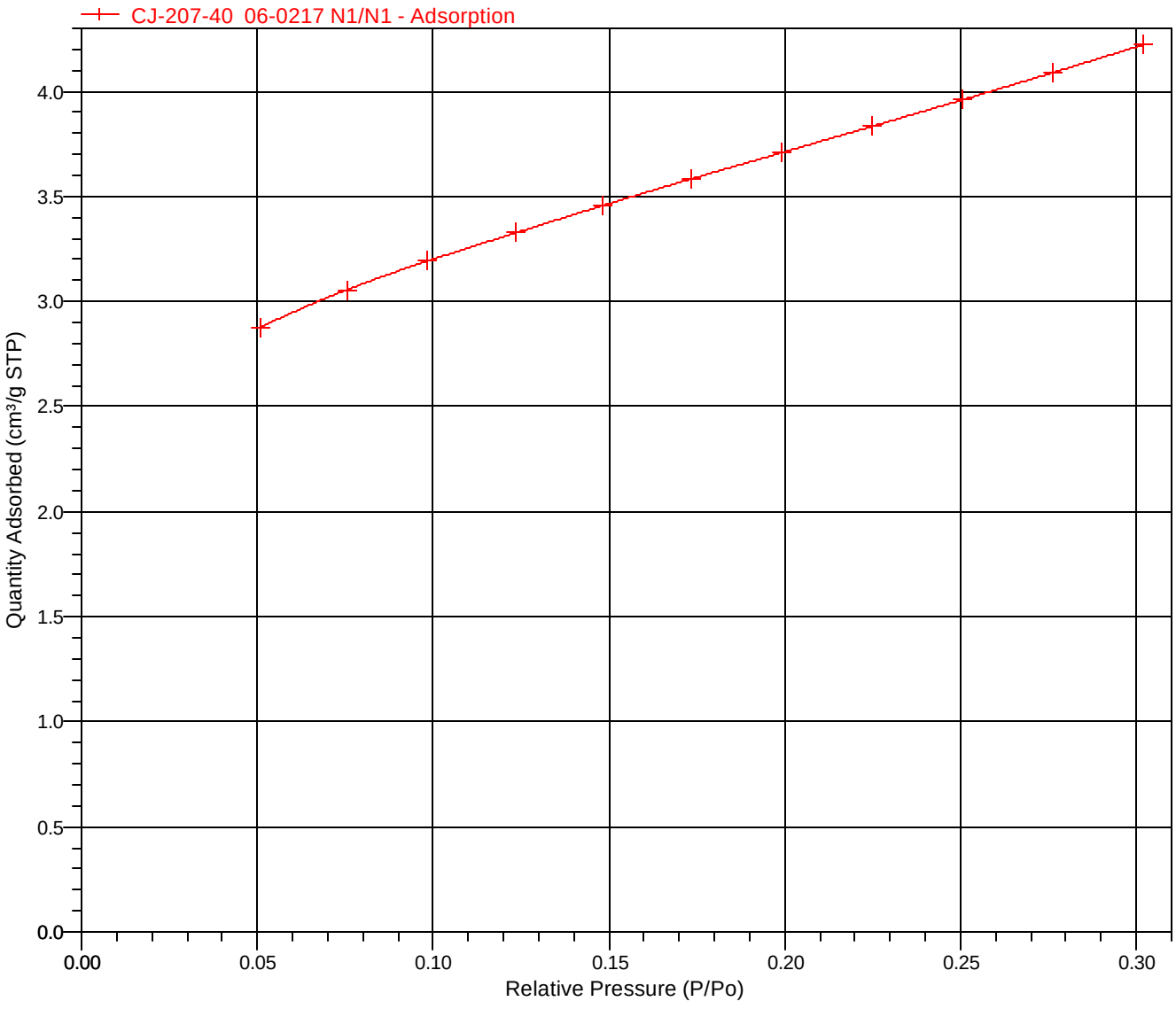
Relative Pressure (P/Po)	Absolute Pressure (mmHg)	Quantity Adsorbed (cm³/g STP)	Elapsed Time (h:min)	Saturation Pressure (mmHg)
			01:08	736.94562
0.051121487	37.68829	2.8779	02:10	
0.075556860	55.71075	3.0562	02:33	
0.098313891	72.49754	3.1924	02:49	
0.123338473	90.95711	3.3267	03:00	
			03:09	737.50061
0.148133515	109.24856	3.4562	03:09	
0.173619345	128.04437	3.5836	03:16	
0.199105163	146.84018	3.7082	03:23	
0.224676473	165.69904	3.8333	03:30	
0.250356073	184.63776	3.9600	03:37	
0.276132543	203.64792	4.0890	03:43	
0.302022993	222.74214	4.2212	03:49	

Sample: CJ-207-40 06-0217 N1/N1
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0217.SMP

Started:	2/1/2006 4:22:41PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 8:12:53PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/2/2006 7:50:36AM	Sample Mass:	4.3543 g
Warm Free Space:	5.5902 cm³ Measured	Cold Free Space:	15.9894 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Linear Plot



Sample: CJ-207-40 06-0217 N1/N1
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0217.SMP

Started: 2/1/2006 4:22:41PM
Completed: 2/1/2006 8:12:53PM
Report Time: 2/2/2006 7:50:36AM
Warm Free Space: 5.5902 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.3543 g
Cold Free Space: 15.9894 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Report

BET Surface Area: 13.1245 ± 0.0495 m²/g
Slope: 0.330055 ± 0.001233 g/cm³ STP
Y-Intercept: 0.001631 ± 0.000219 g/cm³ STP
C: 203.384811
Qm: 3.0149 cm³/g STP
Correlation Coefficient: 0.9999442
Molecular Cross-Sectional Area: 0.1620 nm²

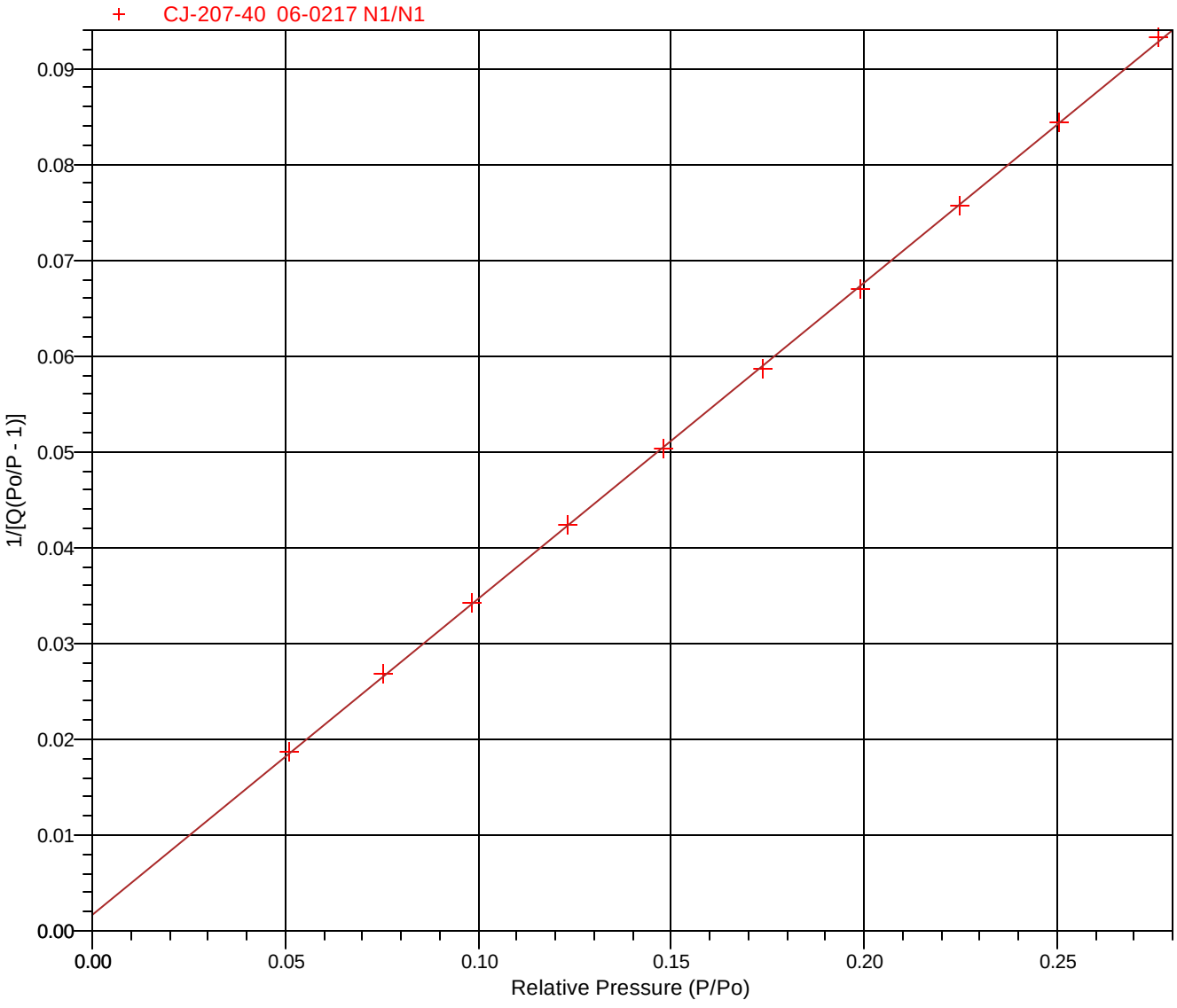
Relative Pressure (P/Po)	Quantity Adsorbed (cm³/g STP)	1/[Q(Po/P - 1)]
0.051121487	2.8779	0.018721
0.075556860	3.0562	0.026743
0.098313891	3.1924	0.034154
0.123338473	3.3267	0.042292
0.148133515	3.4562	0.050313
0.173619345	3.5836	0.058627
0.199105163	3.7082	0.067041
0.224676473	3.8333	0.075597
0.250356073	3.9600	0.084335
0.276132543	4.0890	0.093290

Sample: CJ-207-40 06-0217 N1/N1
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0217.SMP

Started:	2/1/2006 4:22:41PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 8:12:53PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/2/2006 7:50:36AM	Sample Mass:	4.3543 g
Warm Free Space:	5.5902 cm³ Measured	Cold Free Space:	15.9894 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Plot



Sample: CJ-207-40 06-0217 N1/N1
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0217.SMP

Started:	2/1/2006 4:22:41PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 8:12:53PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/2/2006 7:50:36AM	Sample Mass:	4.3543 g
Warm Free Space:	5.5902 cm³ Measured	Cold Free Space:	15.9894 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Summary Report

Surface Area

Single point surface area at P/Po = 0.276132543: 12.8851 m²/g

BET Surface Area: 13.1245 m²/g

Sample: CJ-206-40 06-0216 F3/F3
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0216.SMP

Started: 2/1/2006 4:22:41PM
Completed: 2/1/2006 8:12:53PM
Report Time: 2/1/2006 8:12:54PM
Warm Free Space: 5.3716 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.8010 g
Cold Free Space: 15.0468 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Tabular Report

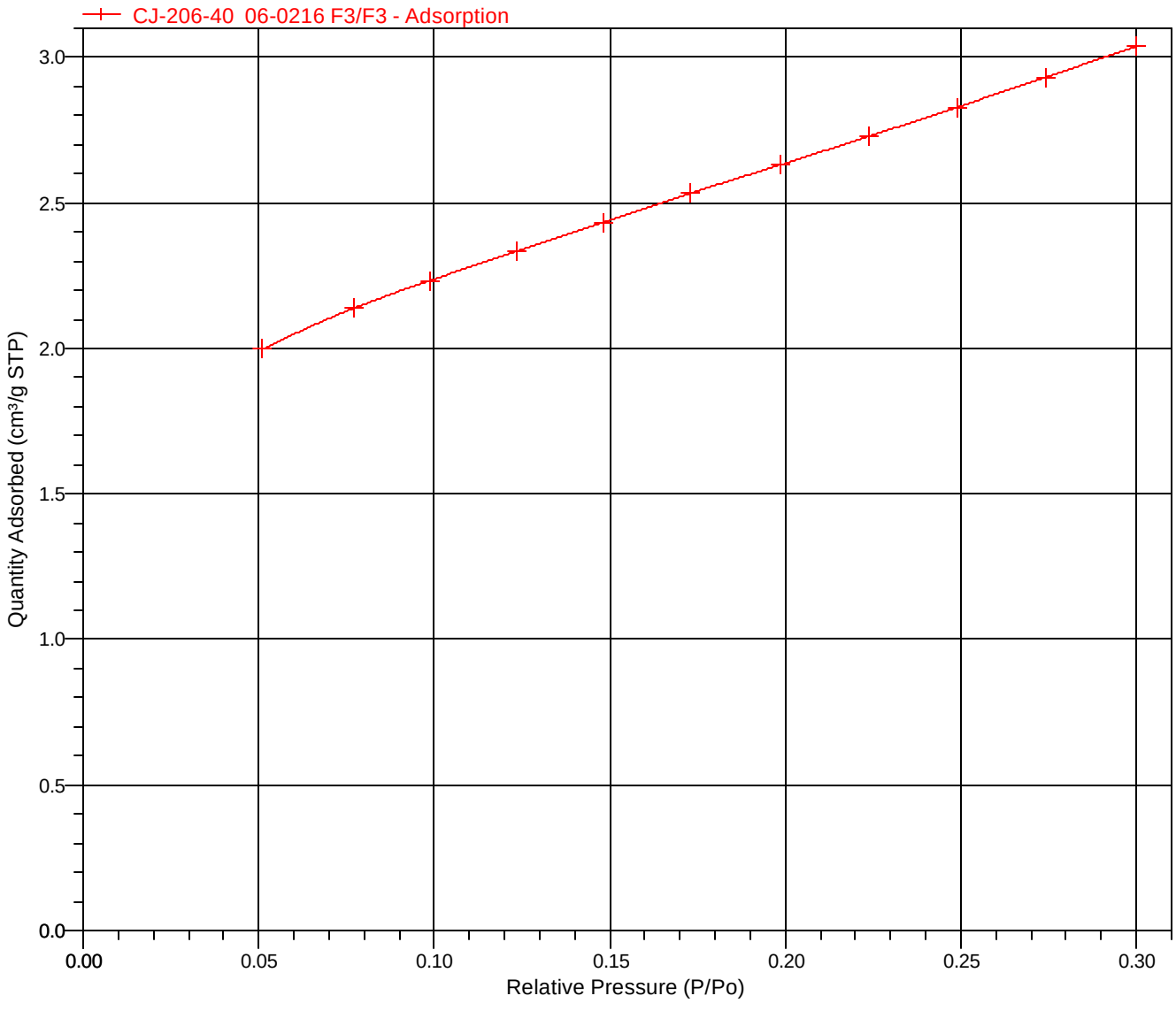
Relative Pressure (P/Po)	Absolute Pressure (mmHg)	Quantity Adsorbed (cm³/g STP)	Elapsed Time (h:min)	Saturation Pressure (mmHg)
			01:08	736.94562
0.050766839	37.41240	1.9969	01:39	
0.077301212	56.96679	2.1382	01:50	
0.098732820	72.76072	2.2335	01:57	
0.123413197	90.94881	2.3341	02:04	
0.147980169	109.05334	2.4337	02:10	
0.172864649	127.39185	2.5332	02:17	
0.198418174	146.22340	2.6309	02:22	
0.223756218	164.89616	2.7288	02:27	
0.248980899	183.48538	2.8292	02:32	
0.274404000	202.22083	2.9321	02:37	
0.300121926	221.17354	3.0374	02:41	

Sample: CJ-206-40 06-0216 F3/F3
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0216.SMP

Started:	2/1/2006 4:22:41PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 8:12:53PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 8:12:54PM	Sample Mass:	4.8010 g
Warm Free Space:	5.3716 cm³ Measured	Cold Free Space:	15.0468 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Linear Plot



Sample: CJ-206-40 06-0216 F3/F3
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0216.SMP

Started: 2/1/2006 4:22:41PM
Completed: 2/1/2006 8:12:53PM
Report Time: 2/1/2006 8:12:54PM
Warm Free Space: 5.3716 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.8010 g
Cold Free Space: 15.0468 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Report

BET Surface Area: 9.4615 ± 0.0195 m²/g
Slope: 0.456311 ± 0.000930 g/cm³ STP
Y-Intercept: 0.003784 ± 0.000178 g/cm³ STP
C: 121.597783
Qm: 2.1735 cm³/g STP
Correlation Coefficient: 0.9999813
Molecular Cross-Sectional Area: 0.1620 nm²

Relative Pressure (P/Po)	Quantity Adsorbed (cm³/g STP)	1/[Q(Po/P - 1)]
0.050766839	1.9969	0.026782
0.077301212	2.1382	0.039182
0.098732820	2.2335	0.049047
0.123413197	2.3341	0.060317
0.147980169	2.4337	0.071364
0.172864649	2.5332	0.082501
0.198418174	2.6309	0.094087
0.223756218	2.7288	0.105634
0.248980899	2.8292	0.117180
0.274404000	2.9321	0.128978
0.300121926	3.0374	0.141178

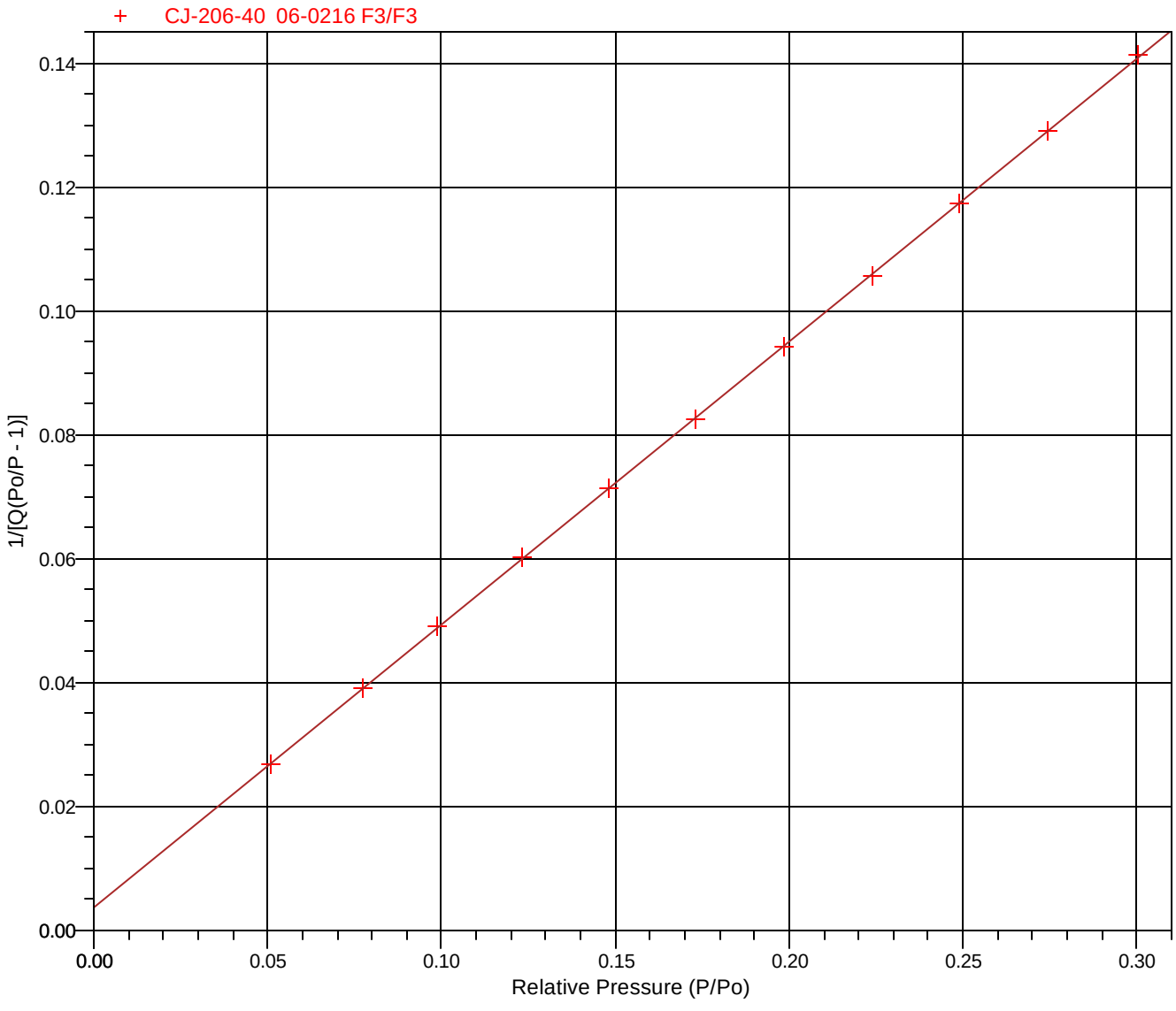
Sample: CJ-206-40 06-0216 F3/F3
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0216.SMP

Started: 2/1/2006 4:22:41PM
Completed: 2/1/2006 8:12:53PM
Report Time: 2/1/2006 8:12:54PM
Warm Free Space: 5.3716 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.8010 g
Cold Free Space: 15.0468 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Plot



Sample: CJ-206-40 06-0216 F3/F3
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0216.SMP

Started: 2/1/2006 4:22:41PM
Completed: 2/1/2006 8:12:53PM
Report Time: 2/1/2006 8:12:54PM
Warm Free Space: 5.3716 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.8010 g
Cold Free Space: 15.0468 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Summary Report

Surface Area

Single point surface area at P/Po = 0.300121926: 9.2542 m²/g

BET Surface Area: 9.4615 m²/g

Sample: CJ-205-40-P 06-0215 G3/G3
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0215.SMP

Started: 2/1/2006 12:24:05PM
Completed: 2/1/2006 3:16:44PM
Report Time: 2/1/2006 3:16:50PM
Warm Free Space: 5.8945 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.4765 g
Cold Free Space: 17.0075 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Tabular Report

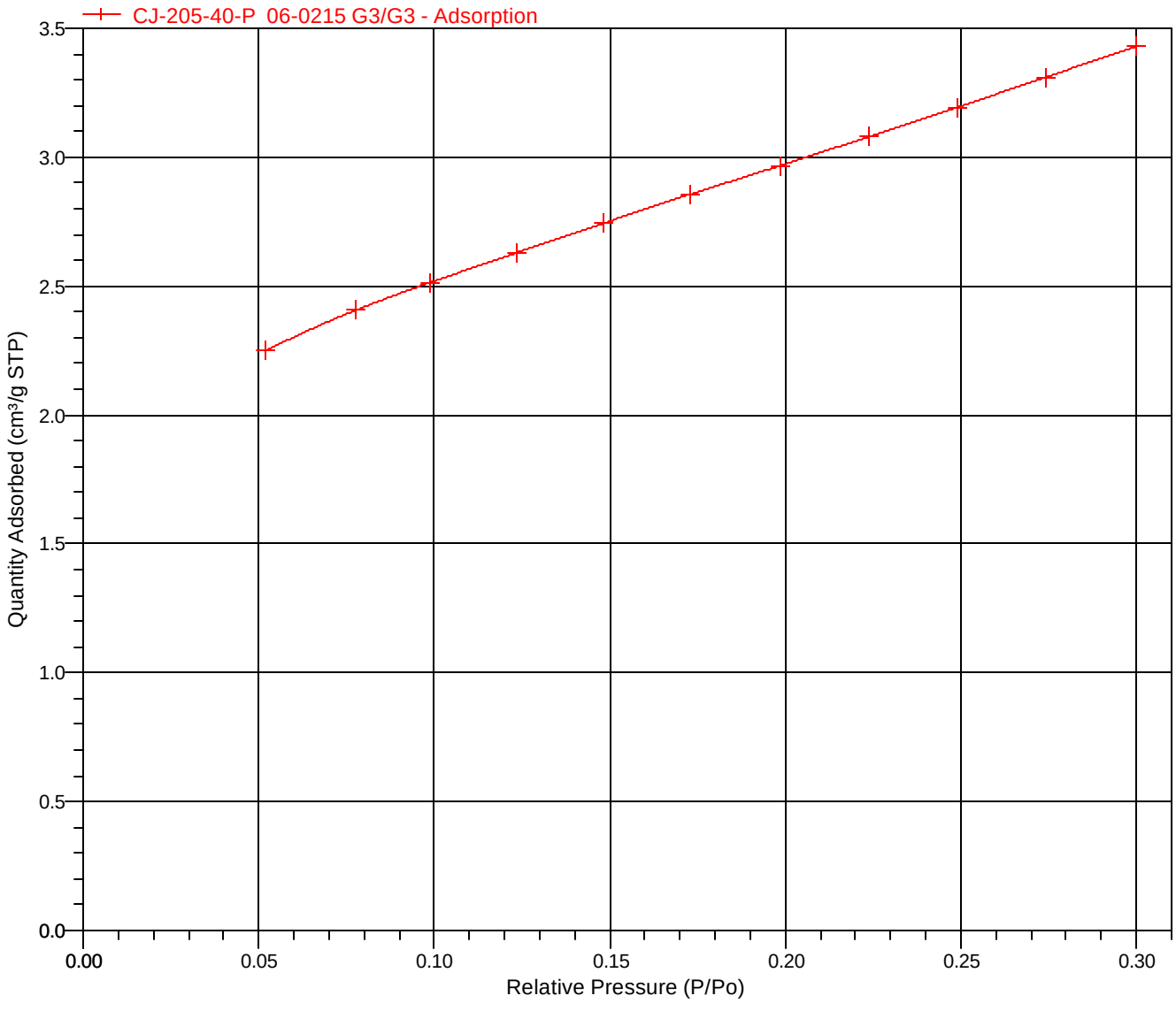
Relative Pressure (P/Po)	Absolute Pressure (mmHg)	Quantity Adsorbed (cm³/g STP)	Elapsed Time (h:min)	Saturation Pressure (mmHg)
			01:13	734.31885
0.051768373	38.01449	2.2498	01:43	
0.077711856	57.06528	2.4063	01:52	
0.098809999	72.55804	2.5137	01:57	
0.123341660	90.57211	2.6296	02:02	
0.148014517	108.68985	2.7437	02:07	
0.173110903	127.11860	2.8561	02:12	
0.198399312	145.68835	2.9674	02:17	
0.223636885	164.22078	3.0796	02:21	
0.249010002	182.85274	3.1938	02:25	
0.274450881	201.53445	3.3106	02:30	
0.300168460	220.41936	3.4299	02:34	

Sample: CJ-205-40-P 06-0215 G3/G3
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0215.SMP

Started:	2/1/2006 12:24:05PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 3:16:44PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 3:16:50PM	Sample Mass:	4.4765 g
Warm Free Space:	5.8945 cm³ Measured	Cold Free Space:	17.0075 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Linear Plot



Sample: CJ-205-40-P 06-0215 G3/G3
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0215.SMP

Started: 2/1/2006 12:24:05PM
Completed: 2/1/2006 3:16:44PM
Report Time: 2/1/2006 3:16:50PM
Warm Free Space: 5.8945 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.4765 g
Cold Free Space: 17.0075 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Report

BET Surface Area: 10.6955 ± 0.0222 m²/g
Slope: 0.403460 ± 0.000830 g/cm³ STP
Y-Intercept: 0.003553 ± 0.000159 g/cm³ STP
C: 114.541452
Qm: 2.4569 cm³/g STP
Correlation Coefficient: 0.9999810
Molecular Cross-Sectional Area: 0.1620 nm²

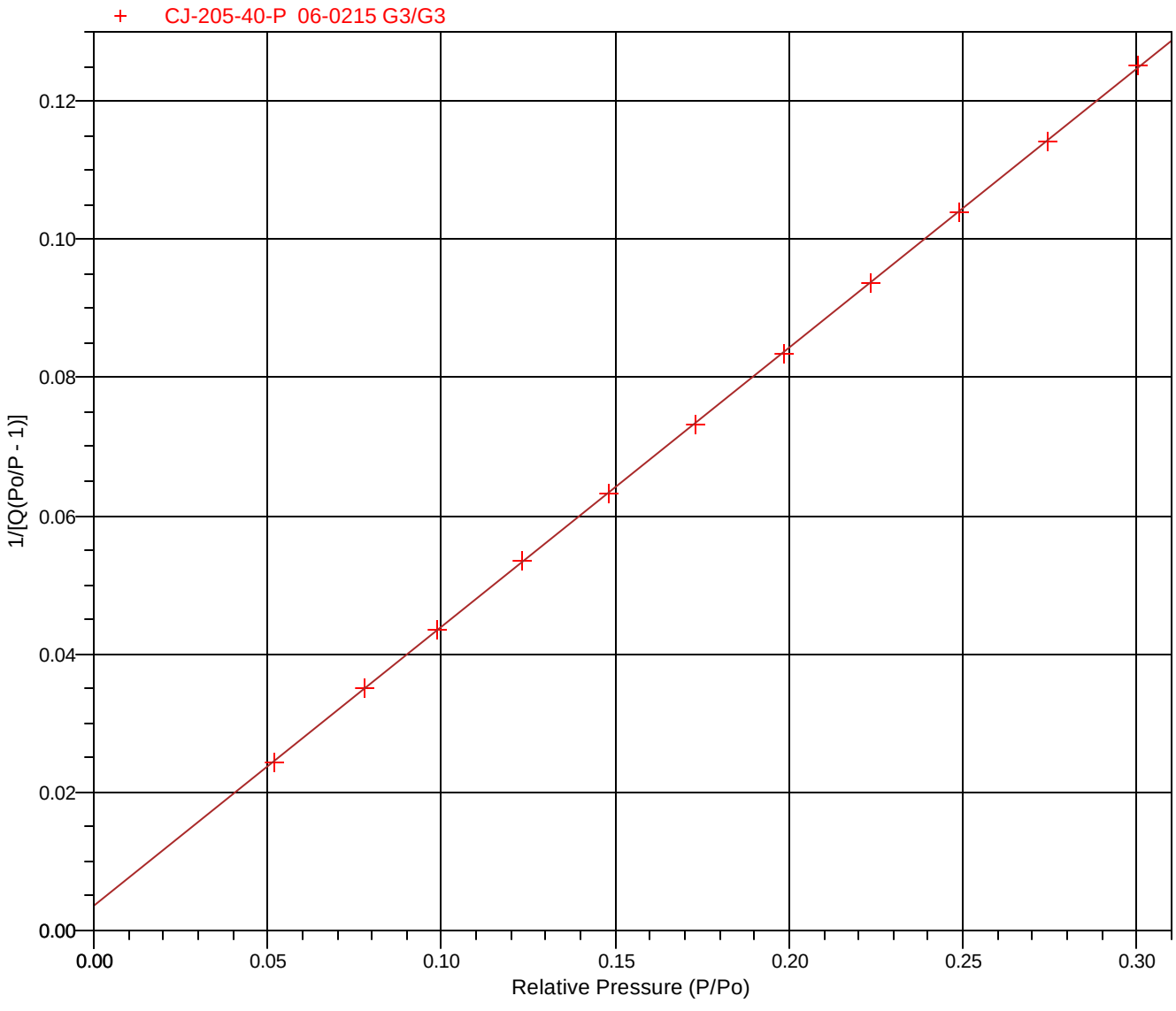
Relative Pressure (P/Po)	Quantity Adsorbed (cm³/g STP)	1/[Q(Po/P - 1)]
0.051768373	2.2498	0.024266
0.077711856	2.4063	0.035016
0.098809999	2.5137	0.043619
0.123341660	2.6296	0.053505
0.148014517	2.7437	0.063319
0.173110903	2.8561	0.073300
0.198399312	2.9674	0.083407
0.223636885	3.0796	0.093537
0.249010002	3.1938	0.103817
0.274450881	3.3106	0.114260
0.300168460	3.4299	0.125050

Sample: CJ-205-40-P 06-0215 G3/G3
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0215.SMP

Started:	2/1/2006 12:24:05PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 3:16:44PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 3:16:50PM	Sample Mass:	4.4765 g
Warm Free Space:	5.8945 cm³ Measured	Cold Free Space:	17.0075 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Plot



Sample: CJ-205-40-P 06-0215 G3/G3
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0215.SMP

Started:	2/1/2006 12:24:05PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 3:16:44PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 3:16:50PM	Sample Mass:	4.4765 g
Warm Free Space:	5.8945 cm³ Measured	Cold Free Space:	17.0075 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Summary Report

Surface Area

Single point surface area at P/Po = 0.300168460: 10.4494 m²/g

BET Surface Area: 10.6955 m²/g

Sample: CJ-201-40 06-0210 3/3
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0210.SMP

Started: 2/1/2006 12:27:55PM
Completed: 2/1/2006 3:23:59PM
Report Time: 2/1/2006 3:24:00PM
Warm Free Space: 5.1716 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.2757 g
Cold Free Space: 14.2717 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Tabular Report

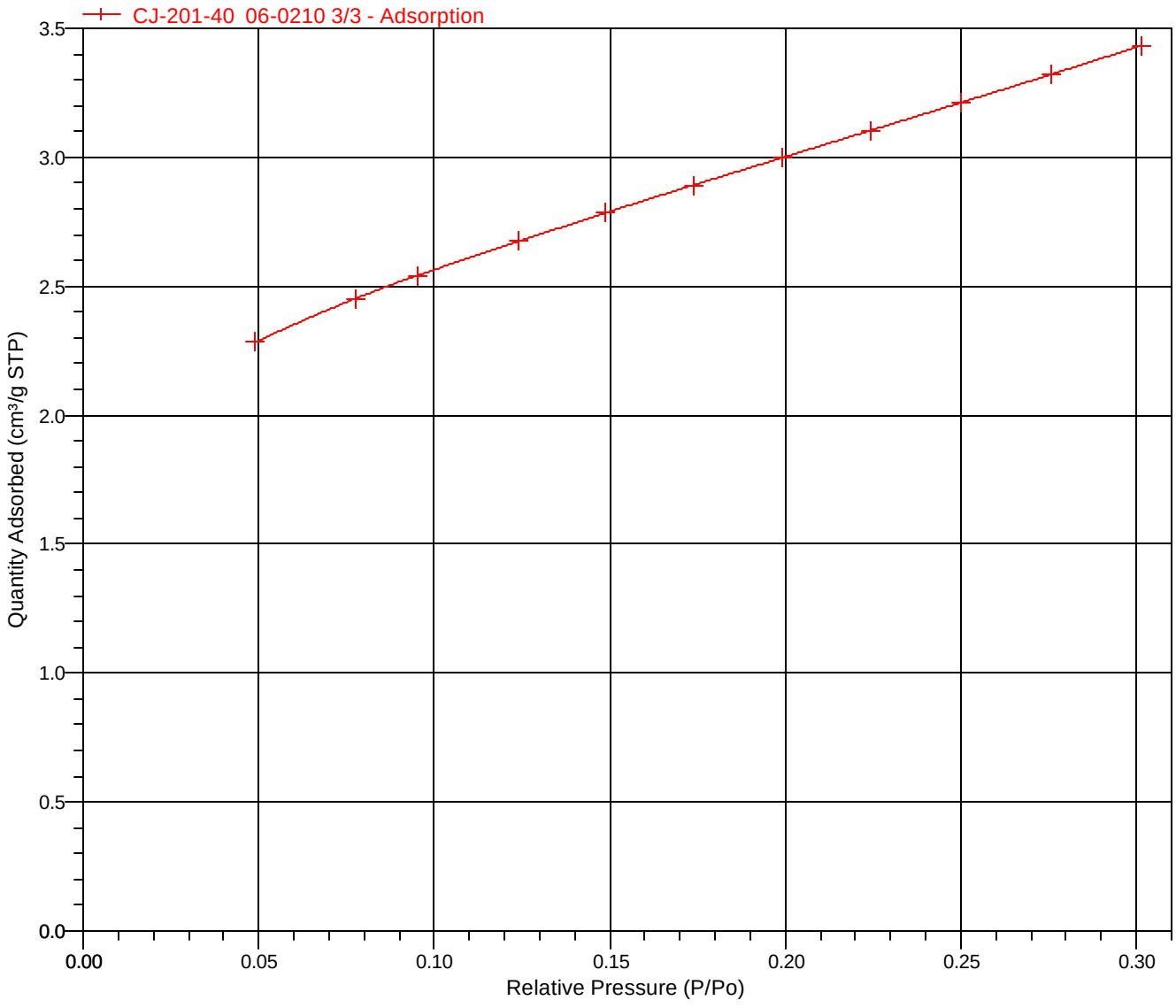
Relative Pressure (P/Po)	Absolute Pressure (mmHg)	Quantity Adsorbed (cm³/g STP)	Elapsed Time (h:min)	Saturation Pressure (mmHg)
			01:10	735.79211
0.048910454	35.98793	2.2822	01:49	
0.077386655	56.94049	2.4522	01:59	
0.095083473	69.96167	2.5421	02:08	
0.123883388	91.15242	2.6734	02:15	
0.148628264	109.35950	2.7840	02:22	
0.173850205	127.91761	2.8924	02:28	
0.199214129	146.58018	2.9983	02:33	
0.224543969	165.21768	3.1044	02:39	
0.250010120	183.95547	3.2120	02:44	
0.275550098	202.74759	3.3213	02:50	
0.301305895	221.69850	3.4329	02:55	

Sample: CJ-201-40 06-0210 3/3
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0210.SMP

Started:	2/1/2006 12:27:55PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 3:23:59PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 3:24:00PM	Sample Mass:	4.2757 g
Warm Free Space:	5.1716 cm³ Measured	Cold Free Space:	14.2717 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Linear Plot



Sample: CJ-201-40 06-0210 3/3
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0210.SMP

Started: 2/1/2006 12:27:55PM
Completed: 2/1/2006 3:23:59PM
Report Time: 2/1/2006 3:24:00PM
Warm Free Space: 5.1716 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.2757 g
Cold Free Space: 14.2717 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Report

BET Surface Area: 10.6561 ± 0.0383 m²/g
Slope: 0.405995 ± 0.001443 g/cm³ STP
Y-Intercept: 0.002523 ± 0.000277 g/cm³ STP
C: 161.941253
Qm: 2.4479 cm³/g STP
Correlation Coefficient: 0.9999432
Molecular Cross-Sectional Area: 0.1620 nm²

Relative Pressure (P/Po)	Quantity Adsorbed (cm³/g STP)	1/[Q(Po/P - 1)]
0.048910454	2.2822	0.022534
0.077386655	2.4522	0.034206
0.095083473	2.5421	0.041333
0.123883388	2.6734	0.052891
0.148628264	2.7840	0.062706
0.173850205	2.8924	0.072755
0.199214129	2.9983	0.082971
0.224543969	3.1044	0.093277
0.250010120	3.2120	0.103784
0.275550098	3.3213	0.114520
0.301305895	3.4329	0.125620

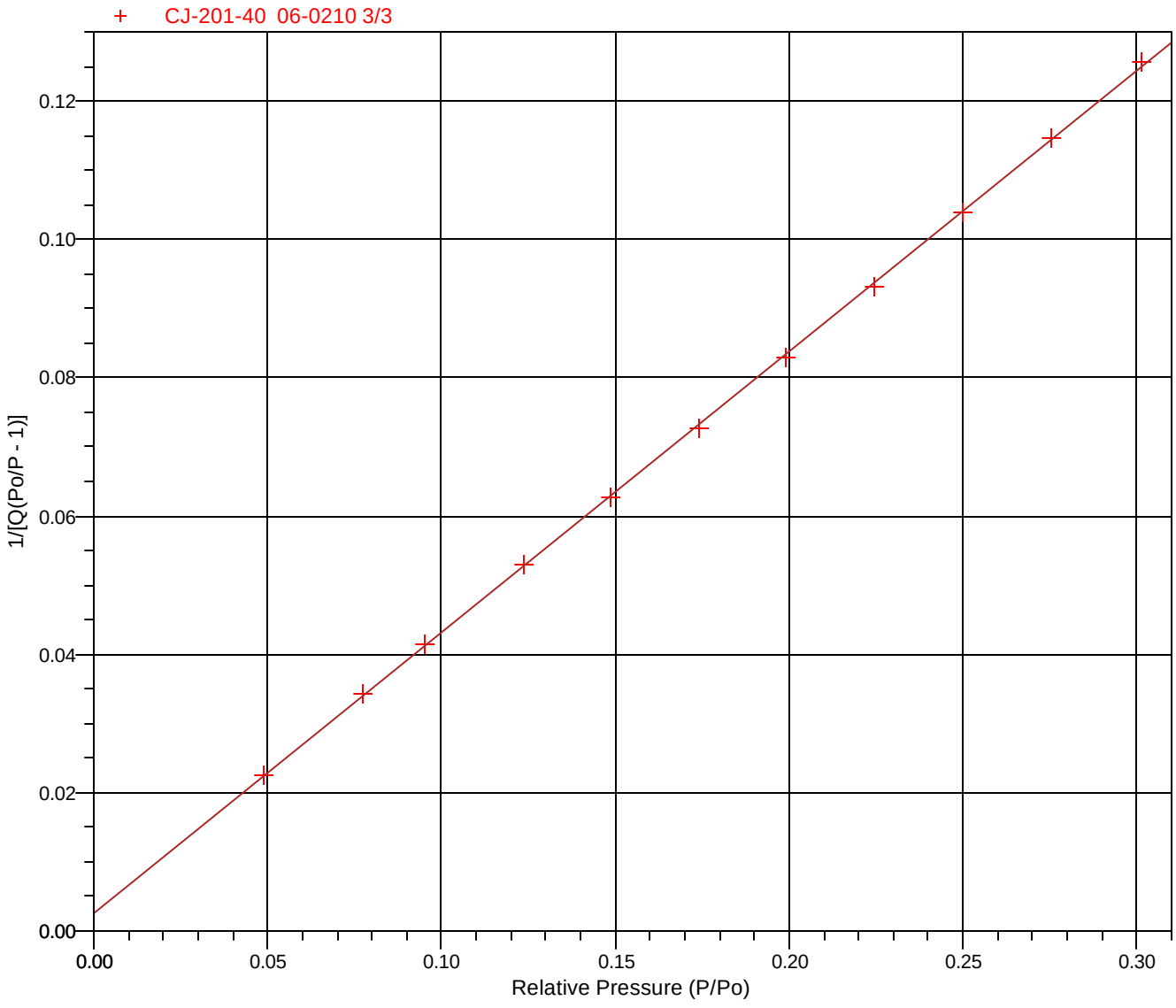
Sample: CJ-201-40 06-0210 3/3
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0210.SMP

Started: 2/1/2006 12:27:55PM
Completed: 2/1/2006 3:23:59PM
Report Time: 2/1/2006 3:24:00PM
Warm Free Space: 5.1716 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.2757 g
Cold Free Space: 14.2717 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Plot



Sample: CJ-201-40 06-0210 3/3
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0210.SMP

Started: 2/1/2006 12:27:55PM
Completed: 2/1/2006 3:23:59PM
Report Time: 2/1/2006 3:24:00PM
Warm Free Space: 5.1716 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.2757 g
Cold Free Space: 14.2717 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Summary Report

Surface Area

Single point surface area at P/Po = 0.301305895: 10.4413 m²/g

BET Surface Area: 10.6561 m²/g

Sample: CJ-202-40 06-0211 38/38
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0211.SMP

Started: 2/1/2006 12:27:55PM
Completed: 2/1/2006 3:23:59PM
Report Time: 2/1/2006 3:42:29PM
Warm Free Space: 6.0917 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.8504 g
Cold Free Space: 17.8637 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Tabular Report

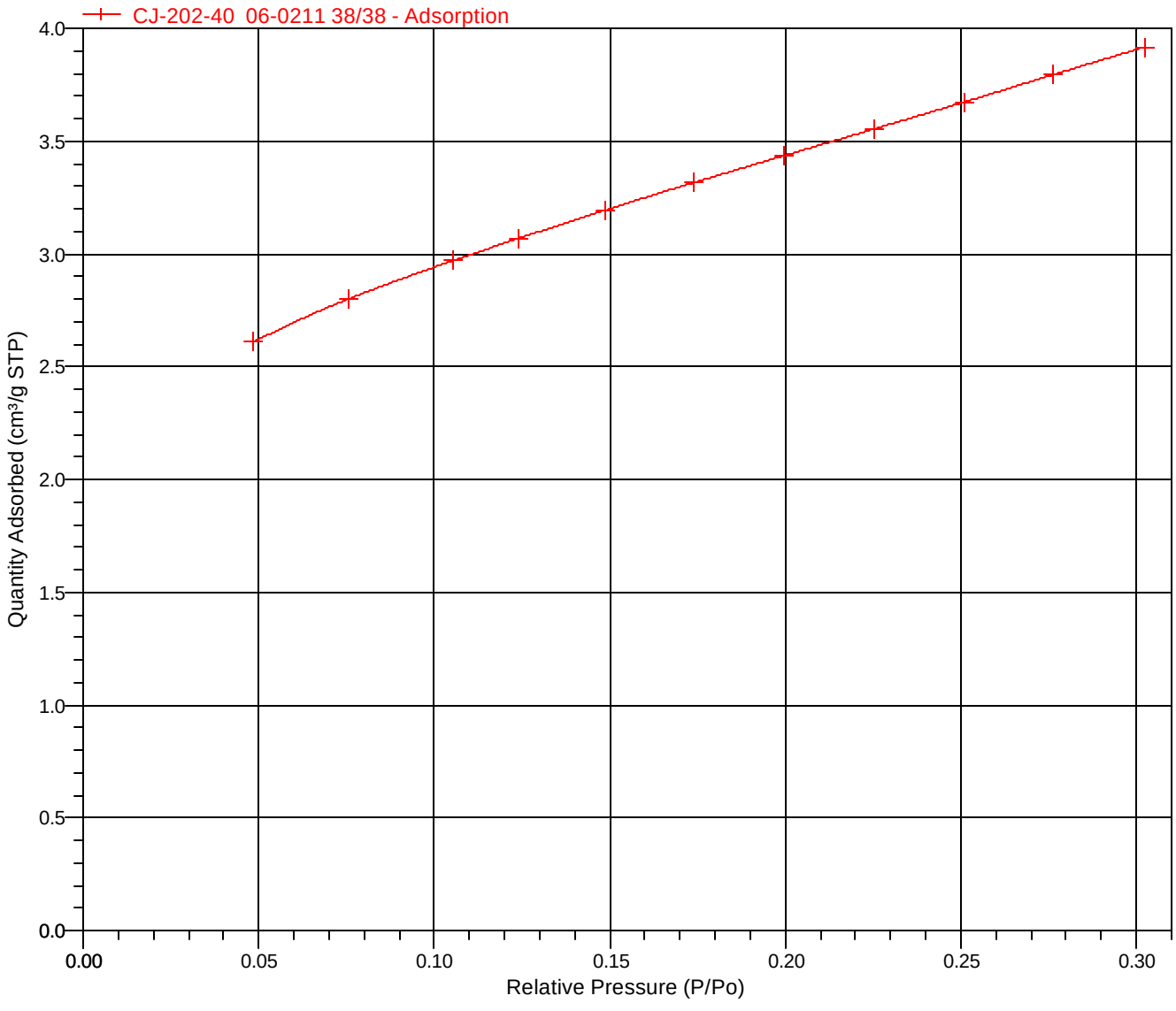
Relative Pressure (P/Po)	Absolute Pressure (mmHg)	Quantity Adsorbed (cm³/g STP)	Elapsed Time (h:min)	Saturation Pressure (mmHg)
			01:10	735.79211
0.048188998	35.45708	2.6084	01:46	
0.075697008	55.69726	2.8007	01:58	
0.105261690	77.45072	2.9694	02:08	
0.124125949	91.33089	3.0685	02:13	
0.148686061	109.40203	3.1933	02:20	
0.174005999	128.03224	3.3160	02:27	
0.199663001	146.91046	3.4353	02:32	
0.225068618	165.60371	3.5540	02:38	
0.250788476	184.52818	3.6731	02:43	
0.276325488	203.31812	3.7943	02:49	
0.302319564	222.44435	3.9175	02:54	

Sample: CJ-202-40 06-0211 38/38
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0211.SMP

Started:	2/1/2006 12:27:55PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 3:23:59PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 3:42:29PM	Sample Mass:	4.8504 g
Warm Free Space:	6.0917 cm³ Measured	Cold Free Space:	17.8637 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Linear Plot



Sample: CJ-202-40 06-0211 38/38
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0211.SMP

Started: 2/1/2006 12:27:55PM
Completed: 2/1/2006 3:23:59PM
Report Time: 2/1/2006 3:42:29PM
Warm Free Space: 6.0917 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.8504 g
Cold Free Space: 17.8637 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Report

BET Surface Area: 12.2117 ± 0.0440 m²/g
Slope: 0.354268 ± 0.001265 g/cm³ STP
Y-Intercept: 0.002211 ± 0.000225 g/cm³ STP
C: 161.265813
Qm: 2.8052 cm³/g STP
Correlation Coefficient: 0.9999490
Molecular Cross-Sectional Area: 0.1620 nm²

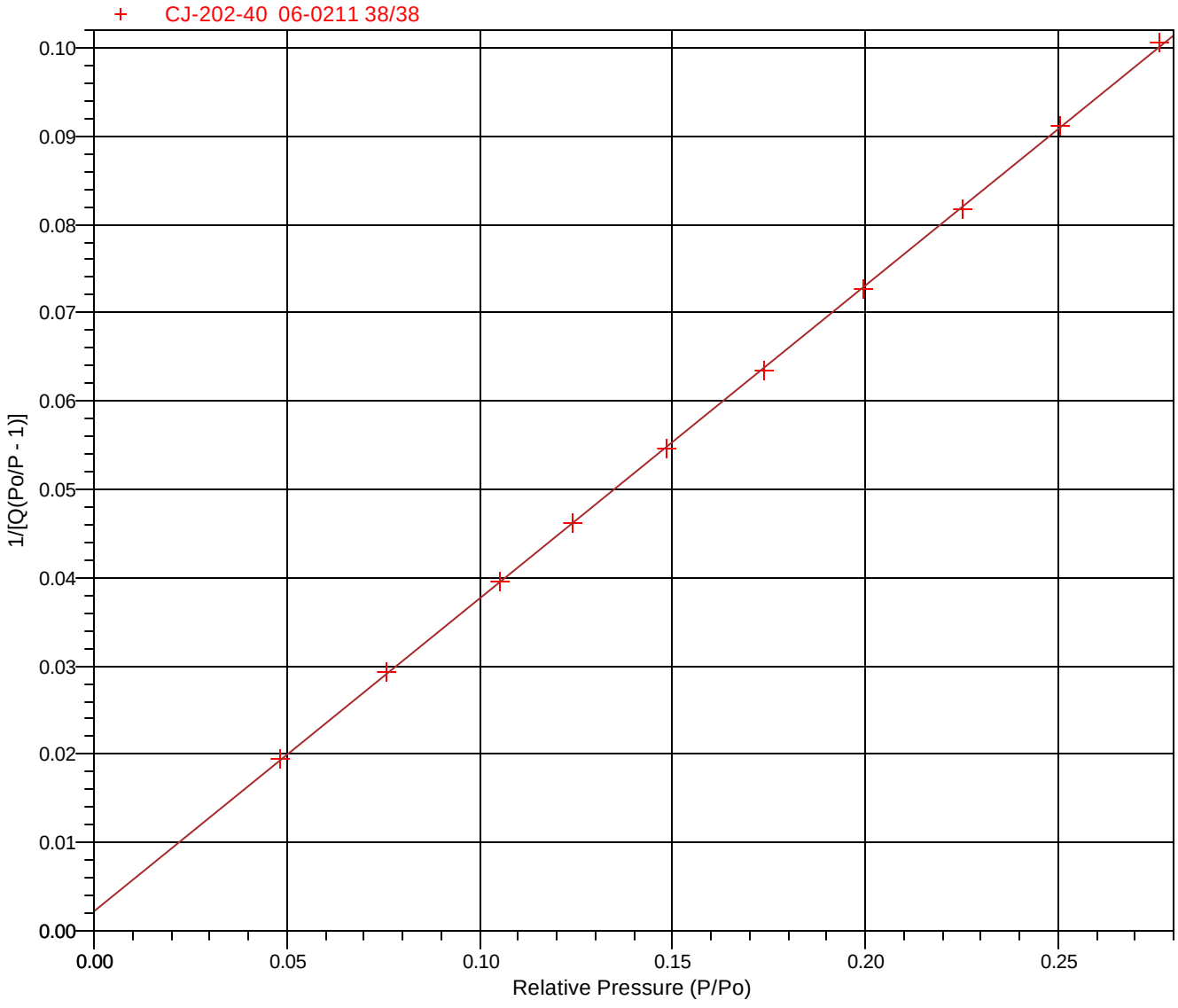
Relative Pressure (P/Po)	Quantity Adsorbed (cm³/g STP)	1/[Q(Po/P - 1)]
0.048188998	2.6084	0.019410
0.075697008	2.8007	0.029241
0.105261690	2.9694	0.039619
0.124125949	3.0685	0.046185
0.148686061	3.1933	0.054694
0.174005999	3.3160	0.063529
0.199663001	3.4353	0.072621
0.225068618	3.5540	0.081722
0.250788476	3.6731	0.091131
0.276325488	3.7943	0.100635

Sample: CJ-202-40 06-0211 38/38
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0211.SMP

Started:	2/1/2006 12:27:55PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 3:23:59PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 3:42:29PM	Sample Mass:	4.8504 g
Warm Free Space:	6.0917 cm³ Measured	Cold Free Space:	17.8637 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Plot



Sample: CJ-202-40 06-0211 38/38
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0211.SMP

Started: 2/1/2006 12:27:55PM
Completed: 2/1/2006 3:23:59PM
Report Time: 2/1/2006 3:42:29PM
Warm Free Space: 6.0917 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.8504 g
Cold Free Space: 17.8637 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Summary Report

Surface Area

Single point surface area at P/Po = 0.276325488: 11.9531 m²/g

BET Surface Area: 12.2117 m²/g

Sample: CJ-203-40 06-0212 815/815
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0212.SMP

Started: 2/1/2006 12:27:55PM
Completed: 2/1/2006 3:23:59PM
Report Time: 2/1/2006 3:24:02PM
Warm Free Space: 5.8383 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.9651 g
Cold Free Space: 16.8406 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Tabular Report

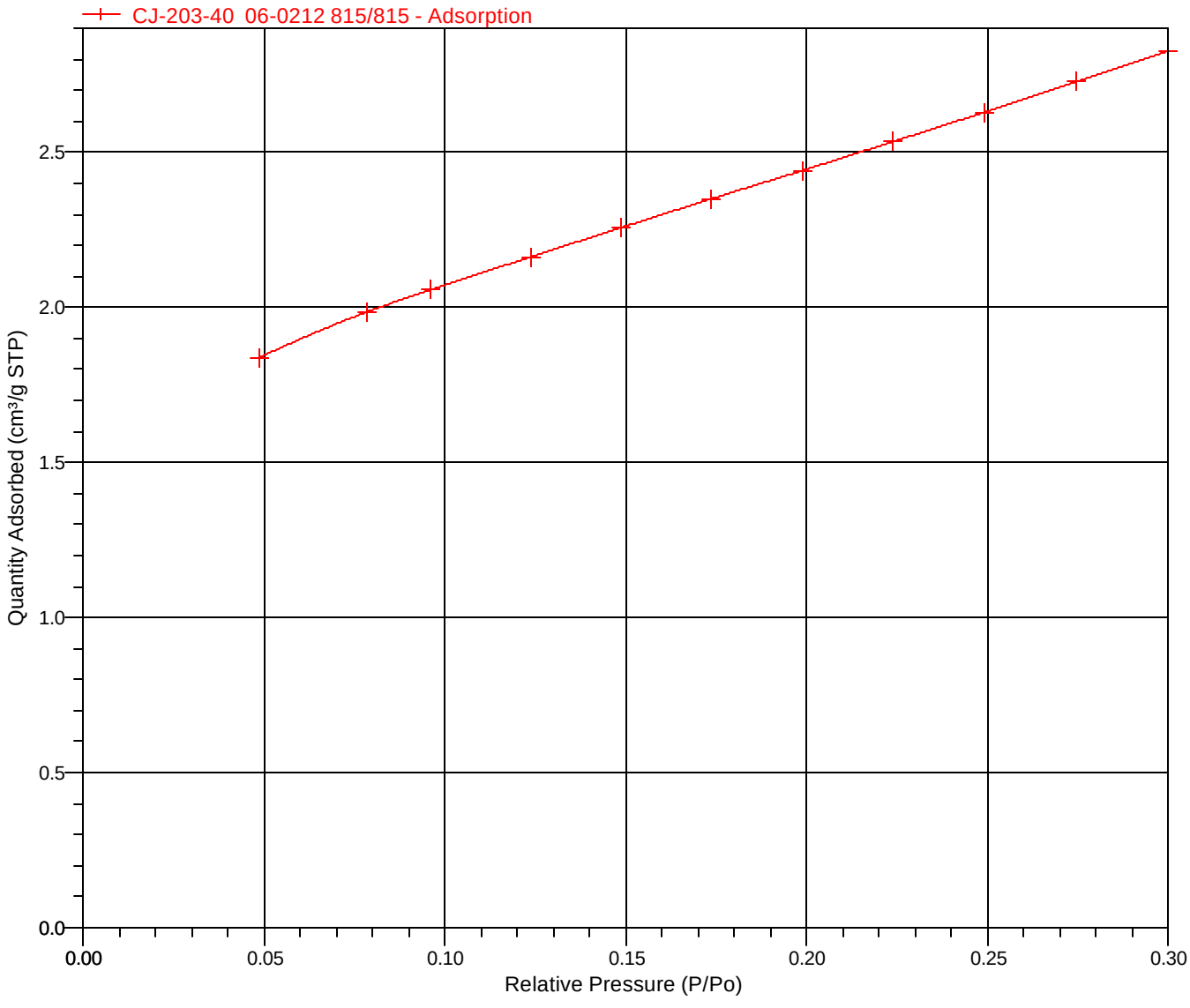
Relative Pressure (P/Po)	Absolute Pressure (mmHg)	Quantity Adsorbed (cm³/g STP)	Elapsed Time (h:min)	Saturation Pressure (mmHg)
			01:10	735.79211
0.048868273	35.95689	1.8390	01:39	
0.078725572	57.92566	1.9854	01:49	
0.095925972	70.58157	2.0561	01:54	
0.123915770	91.17625	2.1632	02:00	
0.148682981	109.39977	2.2569	02:06	
0.173643780	127.76572	2.3496	02:11	
0.198912019	146.35789	2.4415	02:16	
0.224032241	164.84116	2.5341	02:22	
0.249180936	183.34537	2.6292	02:26	
0.274443482	201.93335	2.7267	02:32	
0.299973650	220.71825	2.8268	02:36	

Sample: CJ-203-40 06-0212 815/815
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0212.SMP

Started:	2/1/2006 12:27:55PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 3:23:59PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 3:24:02PM	Sample Mass:	4.9651 g
Warm Free Space:	5.8383 cm³ Measured	Cold Free Space:	16.8406 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Linear Plot



Sample: CJ-203-40 06-0212 815/815
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0212.SMP

Started: 2/1/2006 12:27:55PM
Completed: 2/1/2006 3:23:59PM
Report Time: 2/1/2006 3:24:02PM
Warm Free Space: 5.8383 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.9651 g
Cold Free Space: 16.8406 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Report

BET Surface Area: 8.8087 ± 0.0164 m²/g
Slope: 0.489798 ± 0.000906 g/cm³ STP
Y-Intercept: 0.004396 ± 0.000173 g/cm³ STP
C: 112.409201
Qm: 2.0235 cm³/g STP
Correlation Coefficient: 0.9999846
Molecular Cross-Sectional Area: 0.1620 nm²

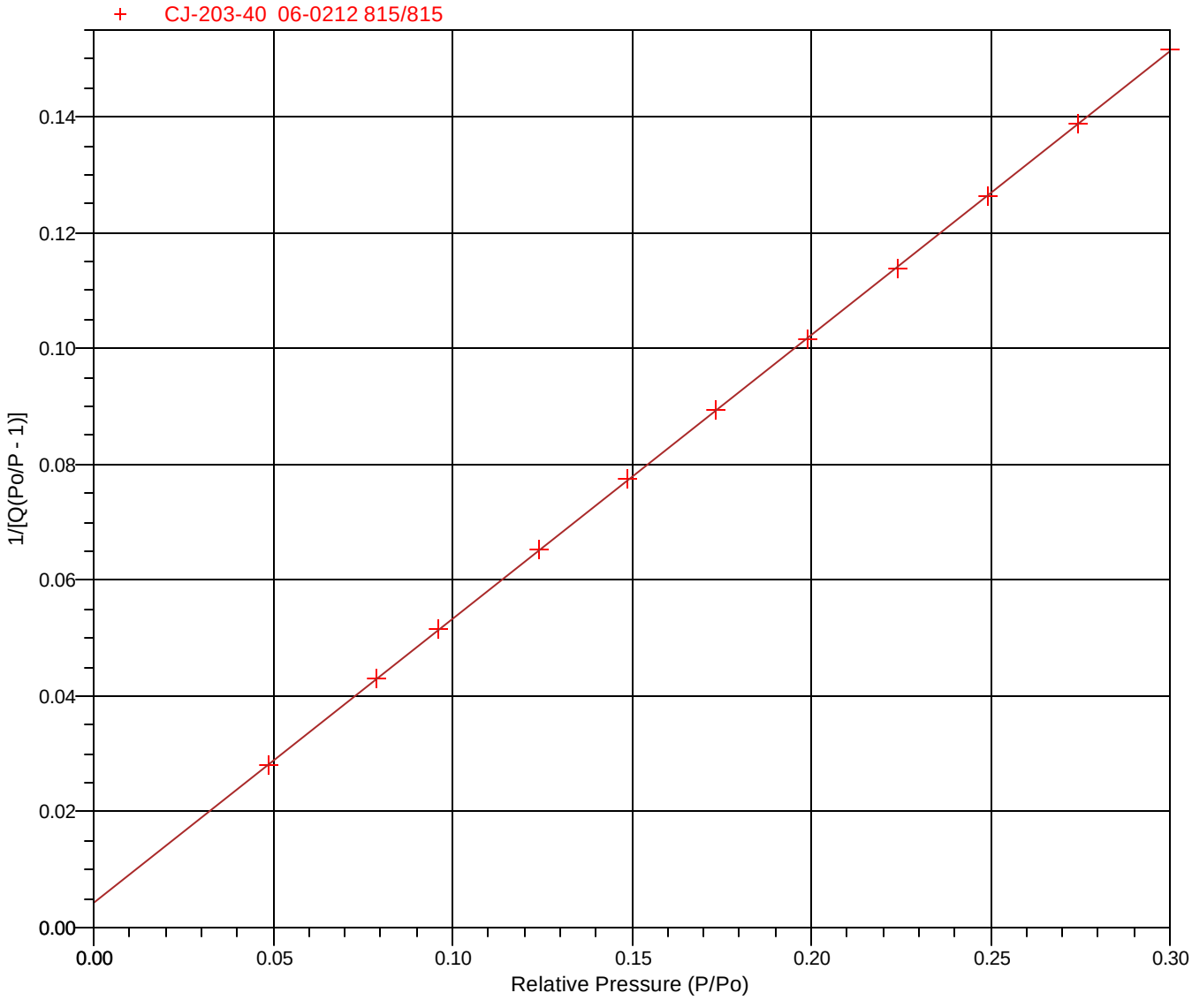
Relative Pressure (P/Po)	Quantity Adsorbed (cm³/g STP)	1/[Q(Po/P - 1)]
0.048868273	1.8390	0.027939
0.078725572	1.9854	0.043041
0.095925972	2.0561	0.051604
0.123915770	2.1632	0.065385
0.148682981	2.2569	0.077385
0.173643780	2.3496	0.089433
0.198912019	2.4415	0.101703
0.224032241	2.5341	0.113929
0.249180936	2.6292	0.126228
0.274443482	2.7267	0.138723
0.299973650	2.8268	0.151593

Sample: CJ-203-40 06-0212 815/815
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0212.SMP

Started:	2/1/2006 12:27:55PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 3:23:59PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 3:24:02PM	Sample Mass:	4.9651 g
Warm Free Space:	5.8383 cm³ Measured	Cold Free Space:	16.8406 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Plot



Sample: CJ-203-40 06-0212 815/815
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0212.SMP

Started:	2/1/2006 12:27:55PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 3:23:59PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 3:24:02PM	Sample Mass:	4.9651 g
Warm Free Space:	5.8383 cm³ Measured	Cold Free Space:	16.8406 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Summary Report

Surface Area

Single point surface area at P/Po = 0.299973650: 8.6142 m²/g

BET Surface Area: 8.8087 m²/g

Sample: CJ-204-40 06-0213 G1/G1
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0213.SMP

Started: 2/1/2006 12:24:05PM
Completed: 2/1/2006 3:16:44PM
Report Time: 2/1/2006 3:43:34PM
Warm Free Space: 5.6492 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.4734 g
Cold Free Space: 16.0508 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Tabular Report

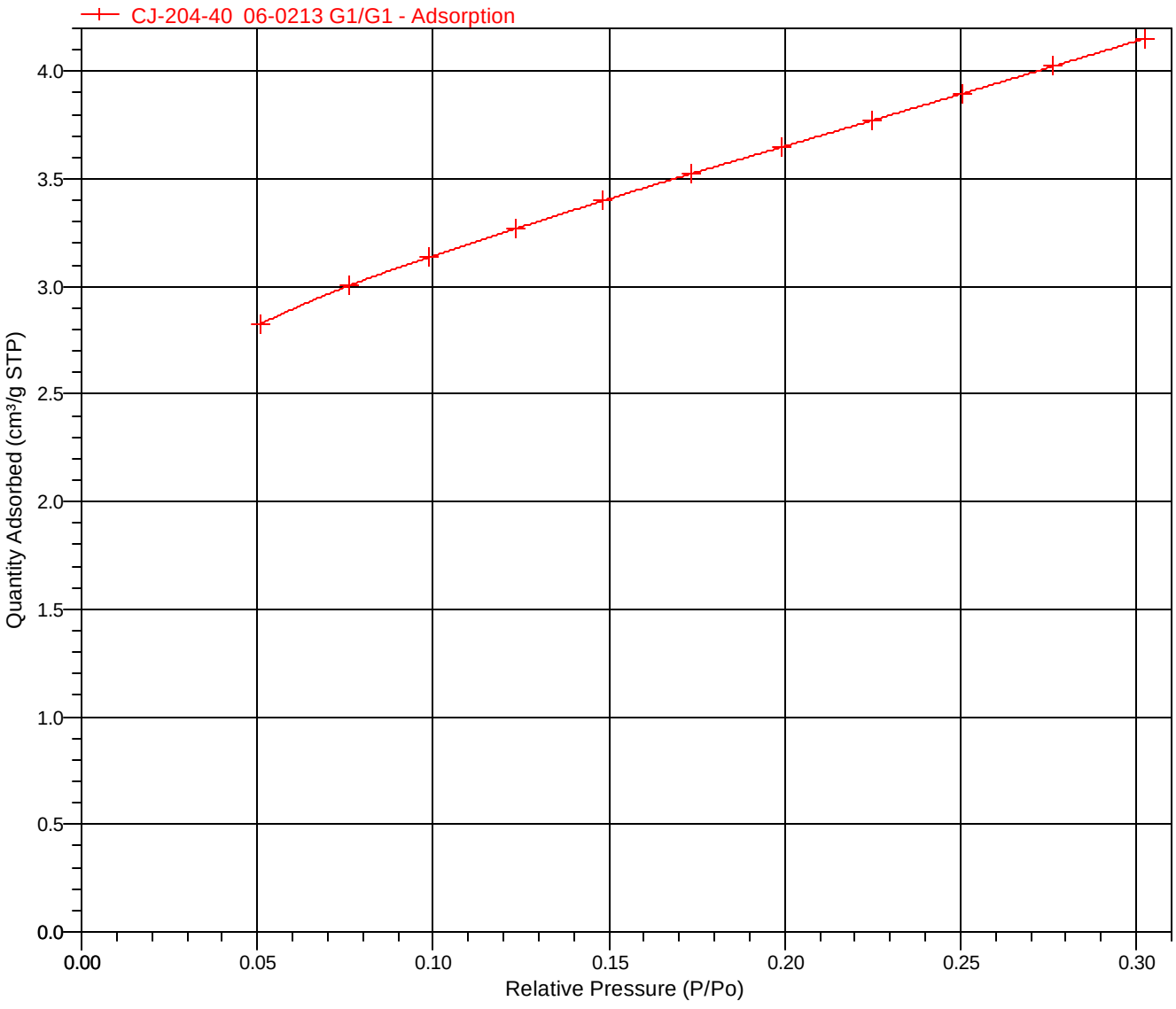
Relative Pressure (P/Po)	Absolute Pressure (mmHg)	Quantity Adsorbed (cm³/g STP)	Elapsed Time (h:min)	Saturation Pressure (mmHg)
			01:13	734.31885
0.051070929	37.50235	2.8265	01:47	
0.076067257	55.85762	3.0041	01:58	
0.098670631	72.45570	3.1361	02:04	
0.123344049	90.57386	3.2685	02:12	
0.148242354	108.85715	3.3977	02:18	
0.173544281	127.43684	3.5242	02:24	
0.199226794	146.29599	3.6479	02:30	
0.224759373	165.04504	3.7714	02:36	
0.250534137	183.97194	3.8965	02:41	
0.276424207	202.98351	4.0230	02:46	
0.302354651	222.02472	4.1525	02:51	

Sample: CJ-204-40 06-0213 G1/G1
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0213.SMP

Started:	2/1/2006 12:24:05PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 3:16:44PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 3:43:34PM	Sample Mass:	4.4734 g
Warm Free Space:	5.6492 cm³ Measured	Cold Free Space:	16.0508 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Linear Plot



Sample: CJ-204-40 06-0213 G1/G1
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0213.SMP

Started: 2/1/2006 12:24:05PM
Completed: 2/1/2006 3:16:44PM
Report Time: 2/1/2006 3:43:34PM
Warm Free Space: 5.6492 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.4734 g
Cold Free Space: 16.0508 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Report

BET Surface Area: 12.9162 ± 0.0501 m²/g
Slope: 0.335315 ± 0.001288 g/cm³ STP
Y-Intercept: 0.001719 ± 0.000229 g/cm³ STP
C: 196.026540
Qm: 2.9671 cm³/g STP
Correlation Coefficient: 0.9999410
Molecular Cross-Sectional Area: 0.1620 nm²

Relative Pressure (P/Po)	Quantity Adsorbed (cm³/g STP)	1/[Q(Po/P - 1)]
0.051070929	2.8265	0.019041
0.076067257	3.0041	0.027406
0.098670631	3.1361	0.034908
0.123344049	3.2685	0.043047
0.148242354	3.3977	0.051223
0.173544281	3.5242	0.059584
0.199226794	3.6479	0.068202
0.224759373	3.7714	0.076873
0.250534137	3.8965	0.085791
0.276424207	4.0230	0.094960

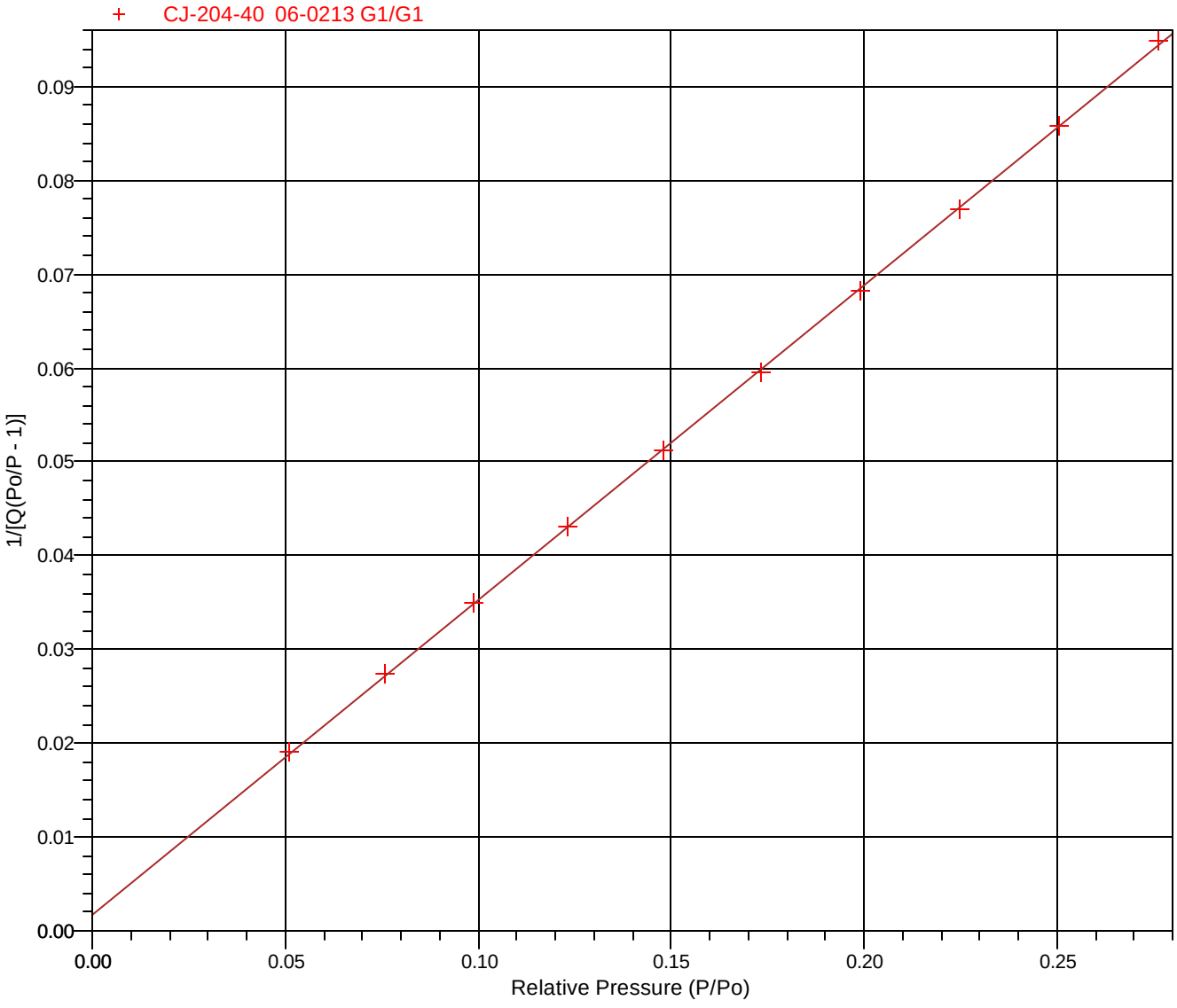
Sample: CJ-204-40 06-0213 G1/G1
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0213.SMP

Started: 2/1/2006 12:24:05PM
Completed: 2/1/2006 3:16:44PM
Report Time: 2/1/2006 3:43:34PM
Warm Free Space: 5.6492 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.4734 g
Cold Free Space: 16.0508 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Plot



Sample: CJ-204-40 06-0213 G1/G1
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0213.SMP

Started: 2/1/2006 12:24:05PM
Completed: 2/1/2006 3:16:44PM
Report Time: 2/1/2006 3:43:34PM
Warm Free Space: 5.6492 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.4734 g
Cold Free Space: 16.0508 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Summary Report

Surface Area

Single point surface area at P/Po = 0.276424207: 12.6720 m²/g

BET Surface Area: 12.9162 m²/g

Sample: CJ-205-40 06-0214 G2/G2
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0214.SMP

Started: 2/1/2006 12:24:05PM
Completed: 2/1/2006 3:16:44PM
Report Time: 2/1/2006 3:16:49PM
Warm Free Space: 5.6027 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.2657 g
Cold Free Space: 15.9013 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Tabular Report

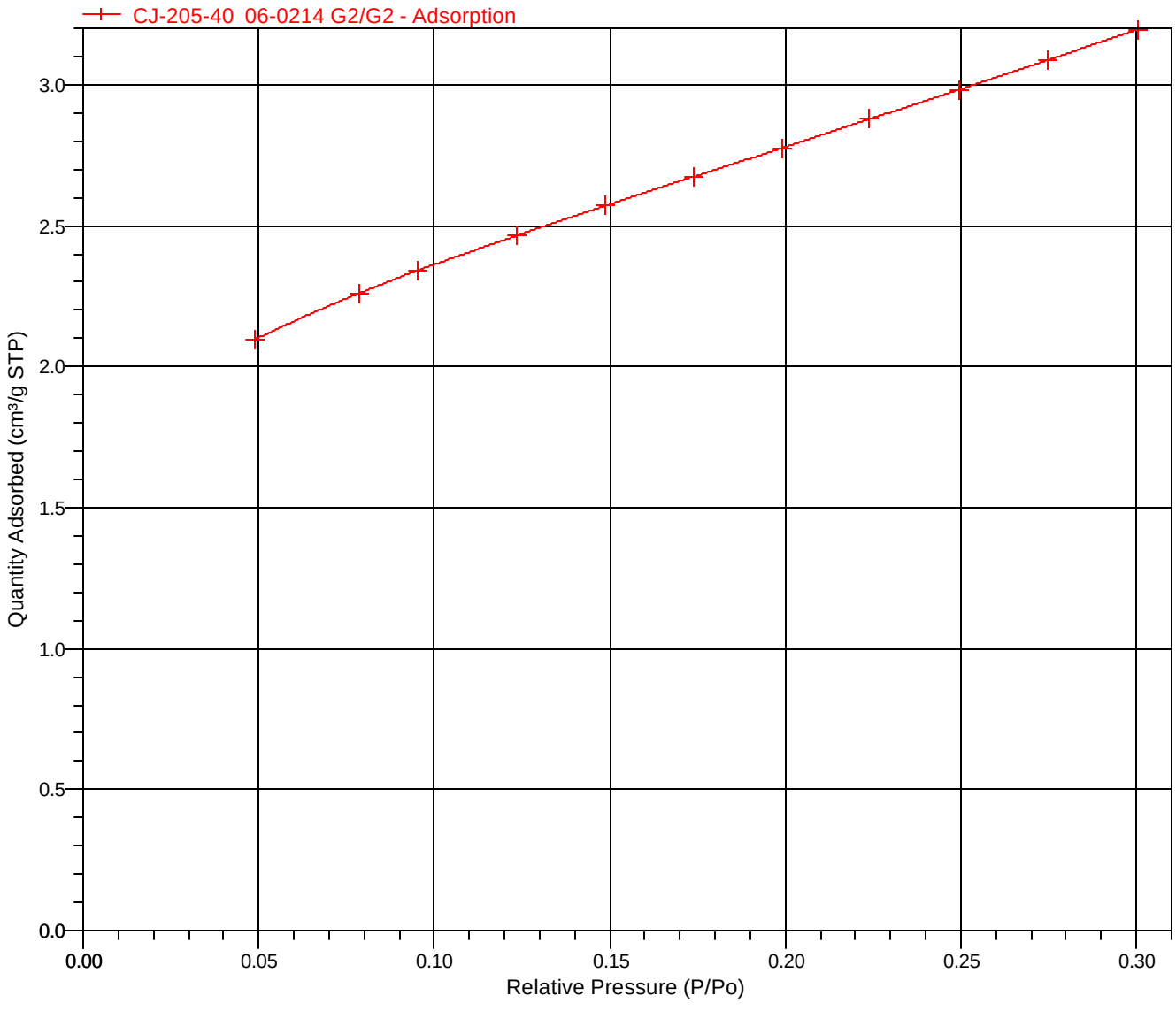
Relative Pressure (P/Po)	Absolute Pressure (mmHg)	Quantity Adsorbed (cm³/g STP)	Elapsed Time (h:min)	Saturation Pressure (mmHg)
			01:13	734.31885
0.049028719	36.00271	2.0965	01:39	
0.078428859	57.59179	2.2602	01:46	
0.095402314	70.05572	2.3412	01:53	
0.123514763	90.69922	2.4647	02:01	
0.148487792	109.03738	2.5710	02:06	
0.173677332	127.53454	2.6739	02:11	
0.198861179	146.02751	2.7753	02:16	
0.224033607	164.51210	2.8776	02:21	
0.249320011	183.08038	2.9817	02:26	
0.274777348	201.77419	3.0875	02:31	
0.300337231	220.54329	3.1959	02:36	

Sample: CJ-205-40 06-0214 G2/G2
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0214.SMP

Started:	2/1/2006 12:24:05PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 3:16:44PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 3:16:49PM	Sample Mass:	4.2657 g
Warm Free Space:	5.6027 cm³ Measured	Cold Free Space:	15.9013 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Linear Plot



Sample: CJ-205-40 06-0214 G2/G2
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0214.SMP

Started: 2/1/2006 12:24:05PM
Completed: 2/1/2006 3:16:44PM
Report Time: 2/1/2006 3:16:49PM
Warm Free Space: 5.6027 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.2657 g
Cold Free Space: 15.9013 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Report

BET Surface Area: 9.9511 ± 0.0246 m²/g
Slope: 0.434049 ± 0.001061 g/cm³ STP
Y-Intercept: 0.003410 ± 0.000203 g/cm³ STP
C: 128.300420
Qm: 2.2859 cm³/g STP
Correlation Coefficient: 0.9999731
Molecular Cross-Sectional Area: 0.1620 nm²

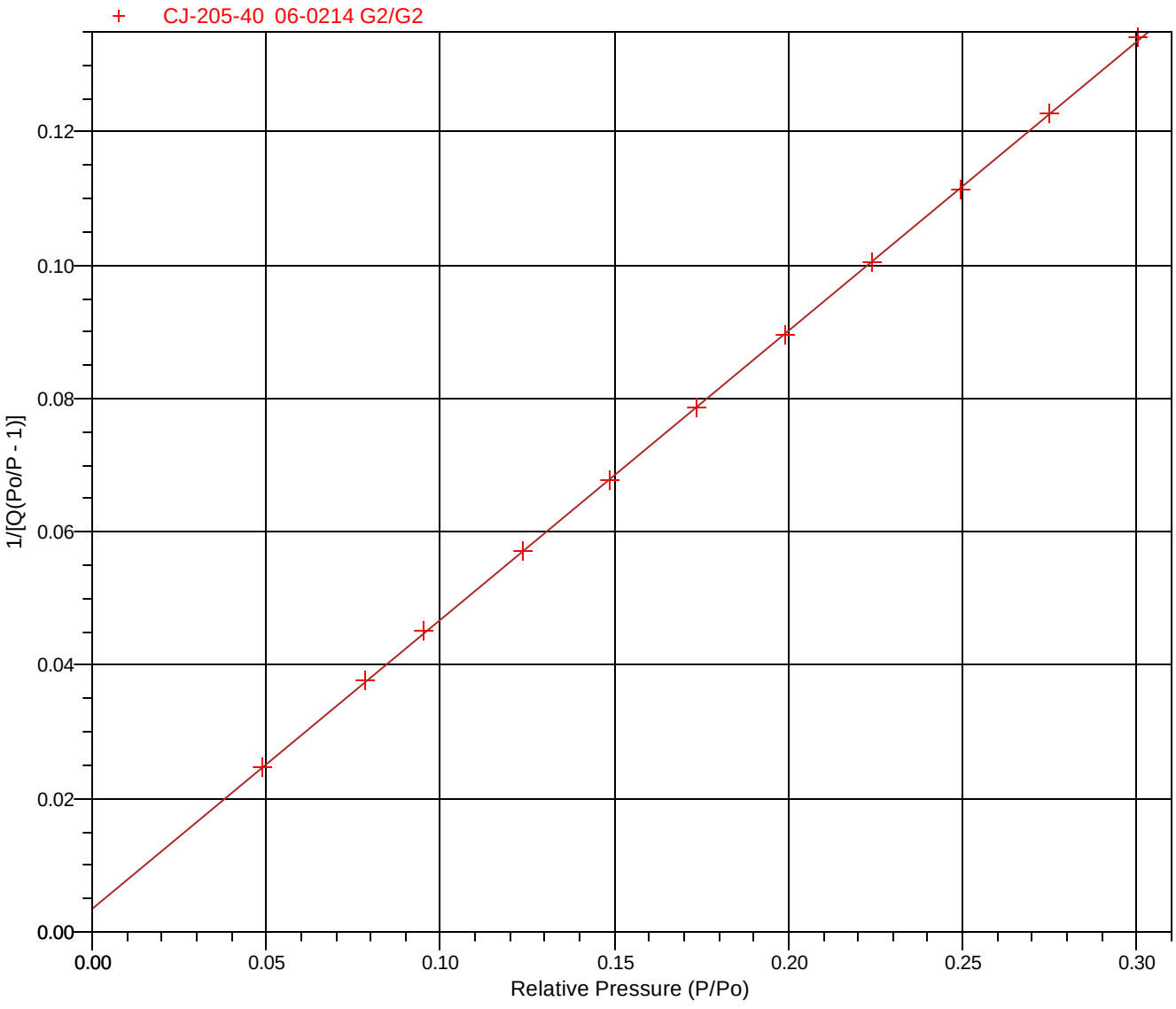
Relative Pressure (P/Po)	Quantity Adsorbed (cm³/g STP)	1/[Q(Po/P - 1)]
0.049028719	2.0965	0.024591
0.078428859	2.2602	0.037652
0.095402314	2.3412	0.045048
0.123514763	2.4647	0.057175
0.148487792	2.5710	0.067826
0.173677332	2.6739	0.078604
0.198861179	2.7753	0.089441
0.224033607	2.8776	0.100333
0.249320011	2.9817	0.111387
0.274777348	3.0875	0.122716
0.300337231	3.1959	0.134314

Sample: CJ-205-40 06-0214 G2/G2
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0214.SMP

Started:	2/1/2006 12:24:05PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 3:16:44PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 3:16:49PM	Sample Mass:	4.2657 g
Warm Free Space:	5.6027 cm³ Measured	Cold Free Space:	15.9013 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Plot



Sample: CJ-205-40 06-0214 G2/G2
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0214.SMP

Started:	2/1/2006 12:24:05PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 3:16:44PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 3:16:49PM	Sample Mass:	4.2657 g
Warm Free Space:	5.6027 cm³ Measured	Cold Free Space:	15.9013 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Summary Report

Surface Area

Single point surface area at P/Po = 0.300337231: 9.7341 m²/g

BET Surface Area: 9.9511 m²/g

Sample: CJ-205-40-P 06-0215 G3/G3
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0215.SMP

Started: 2/1/2006 12:24:05PM
Completed: 2/1/2006 3:16:44PM
Report Time: 2/1/2006 3:16:50PM
Warm Free Space: 5.8945 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.4765 g
Cold Free Space: 17.0075 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Tabular Report

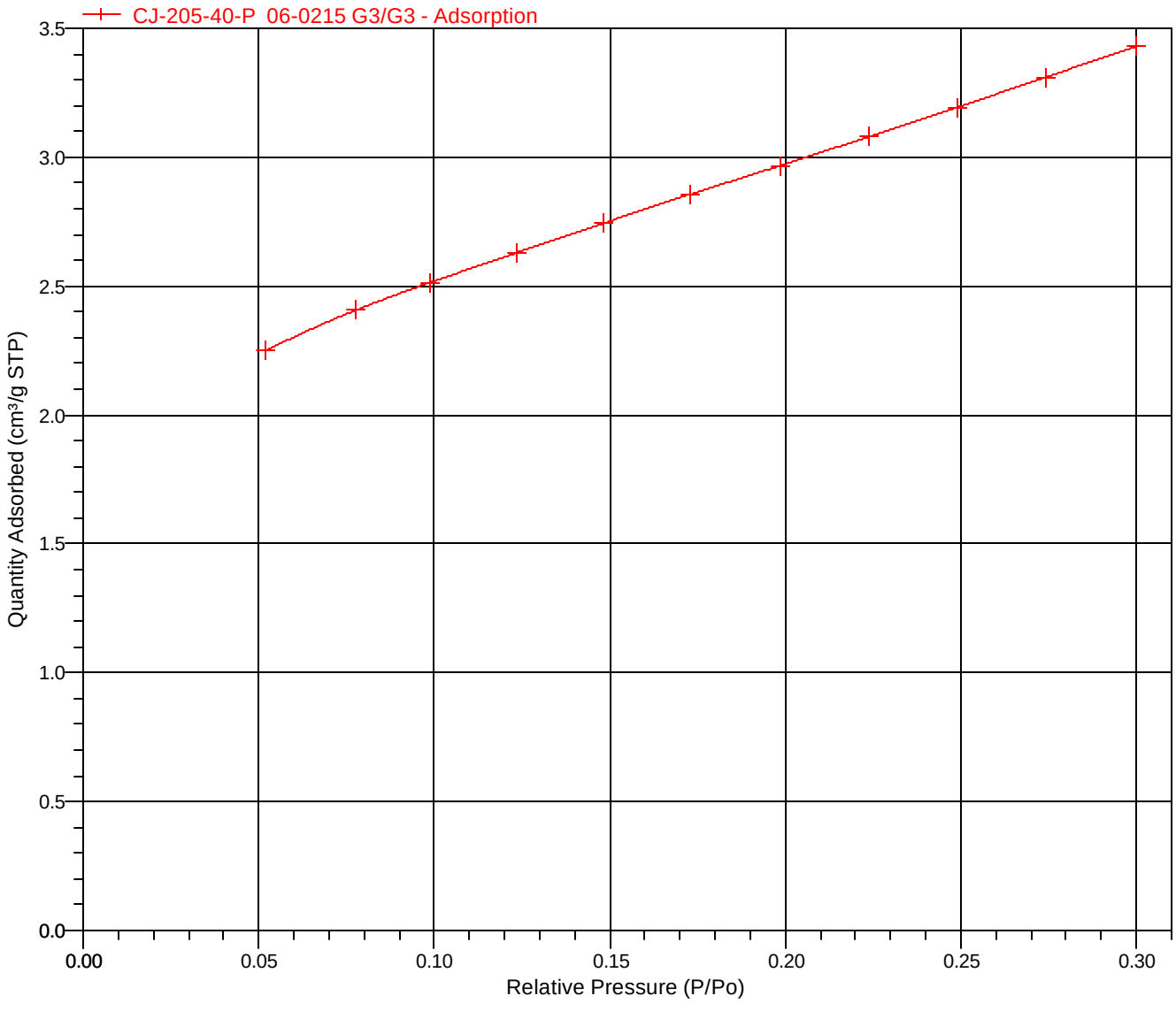
Relative Pressure (P/Po)	Absolute Pressure (mmHg)	Quantity Adsorbed (cm³/g STP)	Elapsed Time (h:min)	Saturation Pressure (mmHg)
			01:13	734.31885
0.051768373	38.01449	2.2498	01:43	
0.077711856	57.06528	2.4063	01:52	
0.098809999	72.55804	2.5137	01:57	
0.123341660	90.57211	2.6296	02:02	
0.148014517	108.68985	2.7437	02:07	
0.173110903	127.11860	2.8561	02:12	
0.198399312	145.68835	2.9674	02:17	
0.223636885	164.22078	3.0796	02:21	
0.249010002	182.85274	3.1938	02:25	
0.274450881	201.53445	3.3106	02:30	
0.300168460	220.41936	3.4299	02:34	

Sample: CJ-205-40-P 06-0215 G3/G3
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0215.SMP

Started:	2/1/2006 12:24:05PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 3:16:44PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 3:16:50PM	Sample Mass:	4.4765 g
Warm Free Space:	5.8945 cm³ Measured	Cold Free Space:	17.0075 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Linear Plot



Sample: CJ-205-40-P 06-0215 G3/G3
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0215.SMP

Started: 2/1/2006 12:24:05PM
Completed: 2/1/2006 3:16:44PM
Report Time: 2/1/2006 3:16:50PM
Warm Free Space: 5.8945 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.4765 g
Cold Free Space: 17.0075 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Report

BET Surface Area: 10.6955 ± 0.0222 m²/g
Slope: 0.403460 ± 0.000830 g/cm³ STP
Y-Intercept: 0.003553 ± 0.000159 g/cm³ STP
C: 114.541452
Qm: 2.4569 cm³/g STP
Correlation Coefficient: 0.9999810
Molecular Cross-Sectional Area: 0.1620 nm²

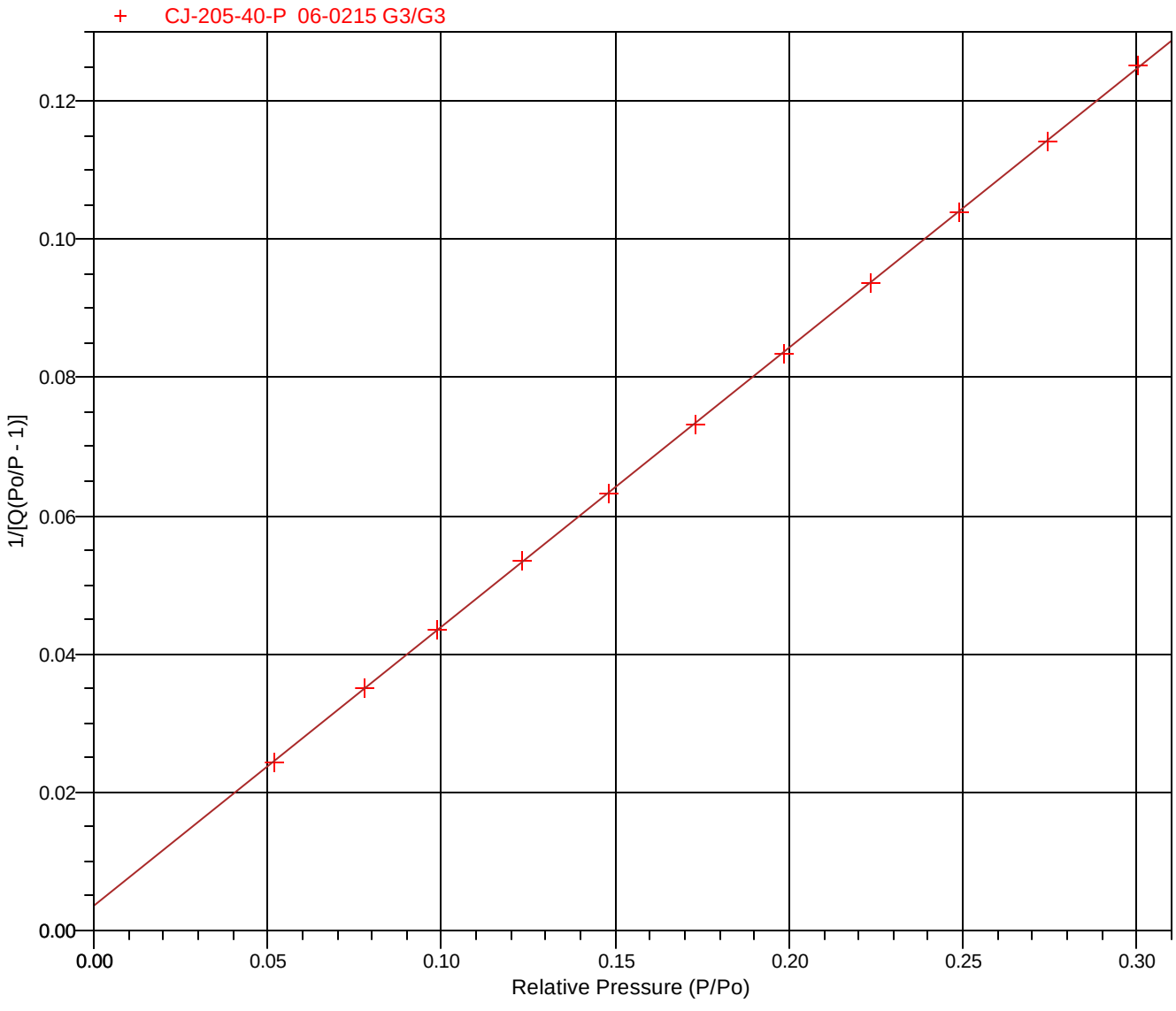
Relative Pressure (P/Po)	Quantity Adsorbed (cm³/g STP)	1/[Q(Po/P - 1)]
0.051768373	2.2498	0.024266
0.077711856	2.4063	0.035016
0.098809999	2.5137	0.043619
0.123341660	2.6296	0.053505
0.148014517	2.7437	0.063319
0.173110903	2.8561	0.073300
0.198399312	2.9674	0.083407
0.223636885	3.0796	0.093537
0.249010002	3.1938	0.103817
0.274450881	3.3106	0.114260
0.300168460	3.4299	0.125050

Sample: CJ-205-40-P 06-0215 G3/G3
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0215.SMP

Started:	2/1/2006 12:24:05PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 3:16:44PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 3:16:50PM	Sample Mass:	4.4765 g
Warm Free Space:	5.8945 cm³ Measured	Cold Free Space:	17.0075 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Plot



Sample: CJ-205-40-P 06-0215 G3/G3
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0215.SMP

Started:	2/1/2006 12:24:05PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 3:16:44PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 3:16:50PM	Sample Mass:	4.4765 g
Warm Free Space:	5.8945 cm³ Measured	Cold Free Space:	17.0075 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Summary Report

Surface Area

Single point surface area at P/Po = 0.300168460: 10.4494 m²/g

BET Surface Area: 10.6955 m²/g

Sample: CJ-206-40 06-0216 F3/F3
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0216.SMP

Started: 2/1/2006 4:22:41PM
Completed: 2/1/2006 8:12:53PM
Report Time: 2/1/2006 8:12:54PM
Warm Free Space: 5.3716 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.8010 g
Cold Free Space: 15.0468 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Tabular Report

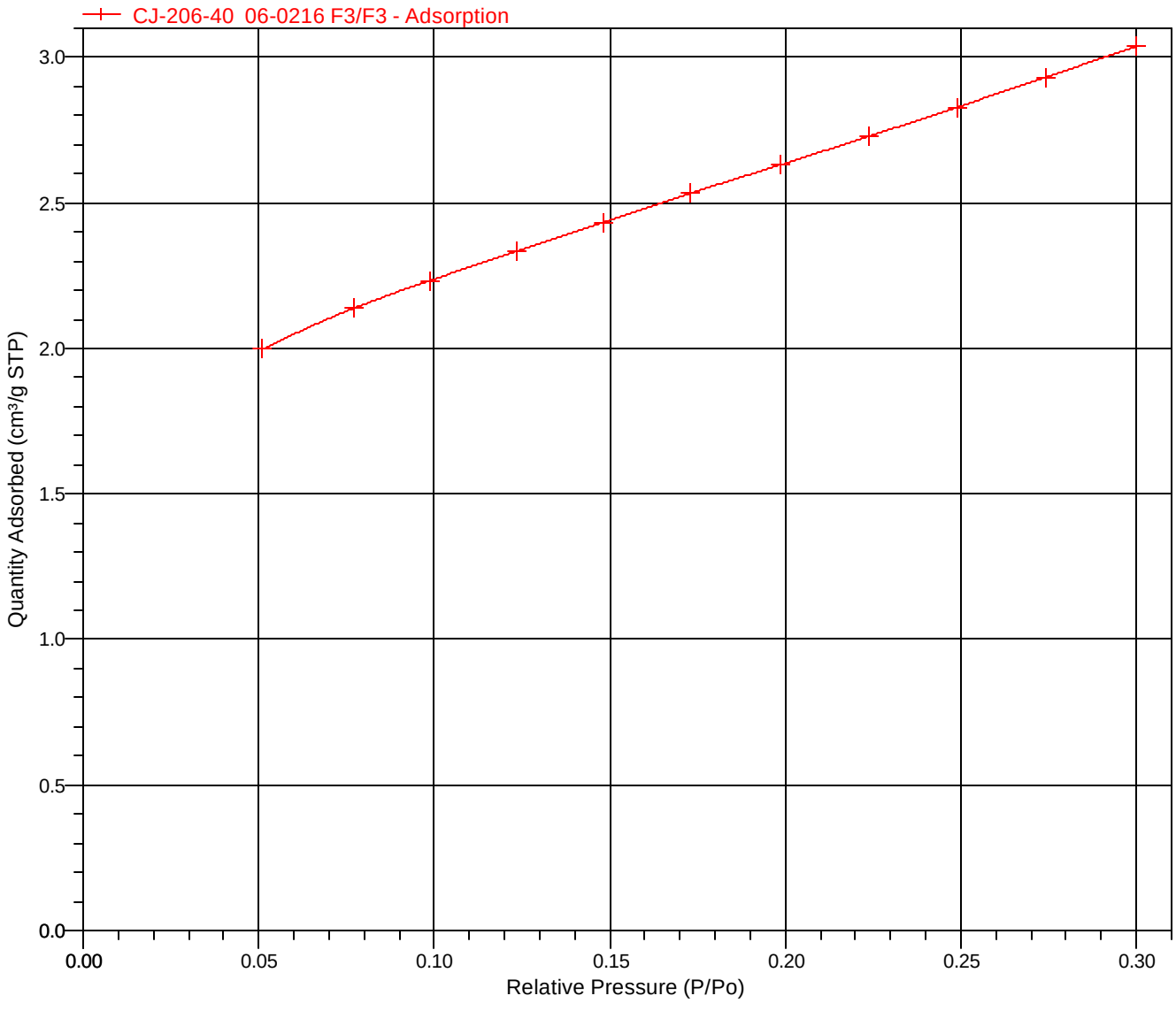
Relative Pressure (P/Po)	Absolute Pressure (mmHg)	Quantity Adsorbed (cm³/g STP)	Elapsed Time (h:min)	Saturation Pressure (mmHg)
			01:08	736.94562
0.050766839	37.41240	1.9969	01:39	
0.077301212	56.96679	2.1382	01:50	
0.098732820	72.76072	2.2335	01:57	
0.123413197	90.94881	2.3341	02:04	
0.147980169	109.05334	2.4337	02:10	
0.172864649	127.39185	2.5332	02:17	
0.198418174	146.22340	2.6309	02:22	
0.223756218	164.89616	2.7288	02:27	
0.248980899	183.48538	2.8292	02:32	
0.274404000	202.22083	2.9321	02:37	
0.300121926	221.17354	3.0374	02:41	

Sample: CJ-206-40 06-0216 F3/F3
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0216.SMP

Started:	2/1/2006 4:22:41PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 8:12:53PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 8:12:54PM	Sample Mass:	4.8010 g
Warm Free Space:	5.3716 cm³ Measured	Cold Free Space:	15.0468 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Linear Plot



Sample: CJ-206-40 06-0216 F3/F3
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0216.SMP

Started: 2/1/2006 4:22:41PM
Completed: 2/1/2006 8:12:53PM
Report Time: 2/1/2006 8:12:54PM
Warm Free Space: 5.3716 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.8010 g
Cold Free Space: 15.0468 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Report

BET Surface Area: 9.4615 ± 0.0195 m²/g
Slope: 0.456311 ± 0.000930 g/cm³ STP
Y-Intercept: 0.003784 ± 0.000178 g/cm³ STP
C: 121.597783
Qm: 2.1735 cm³/g STP
Correlation Coefficient: 0.9999813
Molecular Cross-Sectional Area: 0.1620 nm²

Relative Pressure (P/Po)	Quantity Adsorbed (cm³/g STP)	1/[Q(Po/P - 1)]
0.050766839	1.9969	0.026782
0.077301212	2.1382	0.039182
0.098732820	2.2335	0.049047
0.123413197	2.3341	0.060317
0.147980169	2.4337	0.071364
0.172864649	2.5332	0.082501
0.198418174	2.6309	0.094087
0.223756218	2.7288	0.105634
0.248980899	2.8292	0.117180
0.274404000	2.9321	0.128978
0.300121926	3.0374	0.141178

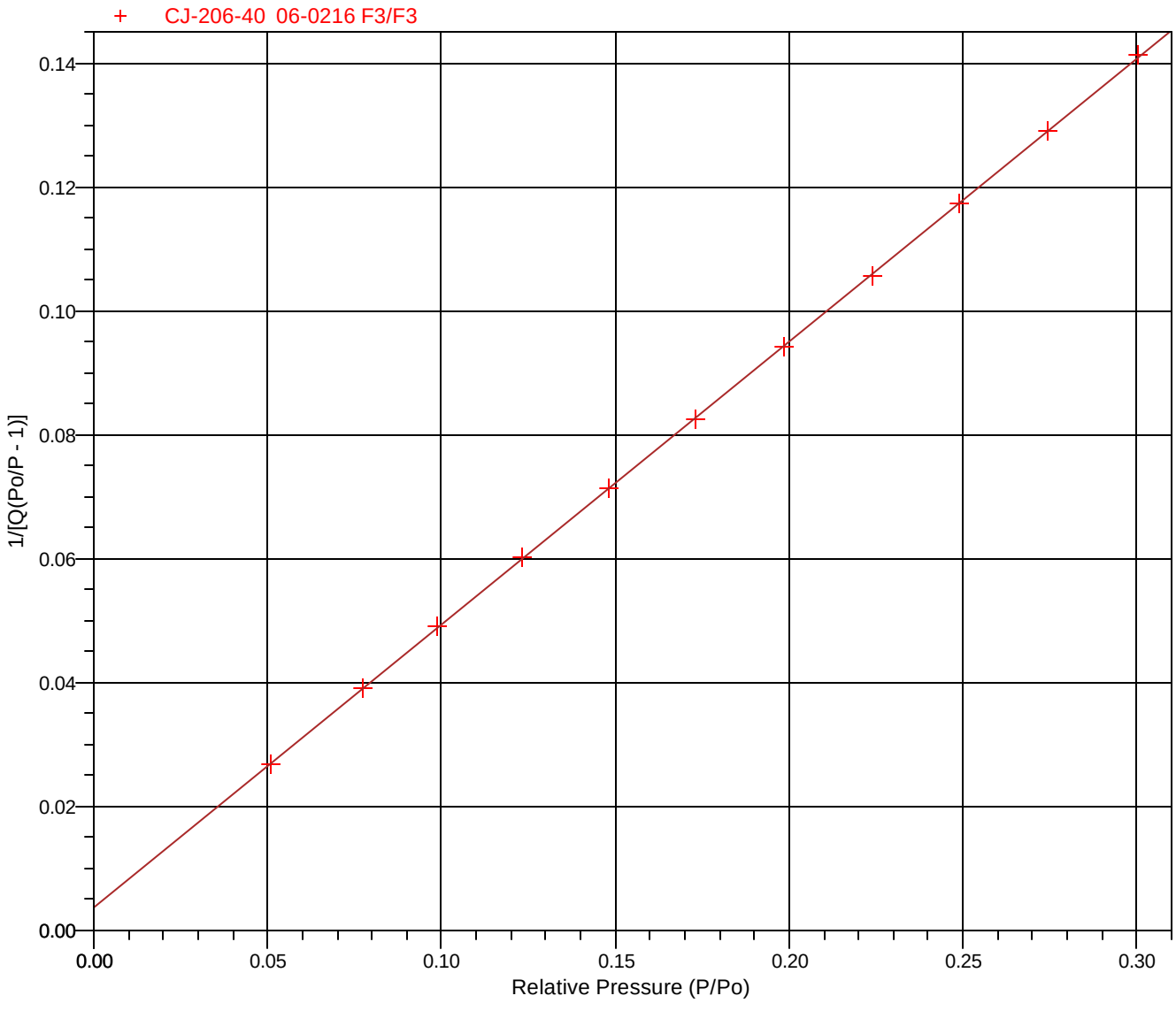
Sample: CJ-206-40 06-0216 F3/F3
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0216.SMP

Started: 2/1/2006 4:22:41PM
Completed: 2/1/2006 8:12:53PM
Report Time: 2/1/2006 8:12:54PM
Warm Free Space: 5.3716 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.8010 g
Cold Free Space: 15.0468 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Plot



Sample: CJ-206-40 06-0216 F3/F3
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0216.SMP

Started: 2/1/2006 4:22:41PM
Completed: 2/1/2006 8:12:53PM
Report Time: 2/1/2006 8:12:54PM
Warm Free Space: 5.3716 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.8010 g
Cold Free Space: 15.0468 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Summary Report

Surface Area

Single point surface area at P/Po = 0.300121926: 9.2542 m²/g

BET Surface Area: 9.4615 m²/g

Sample: CJ-207-40 06-0217 N1/N1
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0217.SMP

Started: 2/1/2006 4:22:41PM
Completed: 2/1/2006 8:12:53PM
Report Time: 2/2/2006 7:50:36AM
Warm Free Space: 5.5902 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.3543 g
Cold Free Space: 15.9894 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Tabular Report

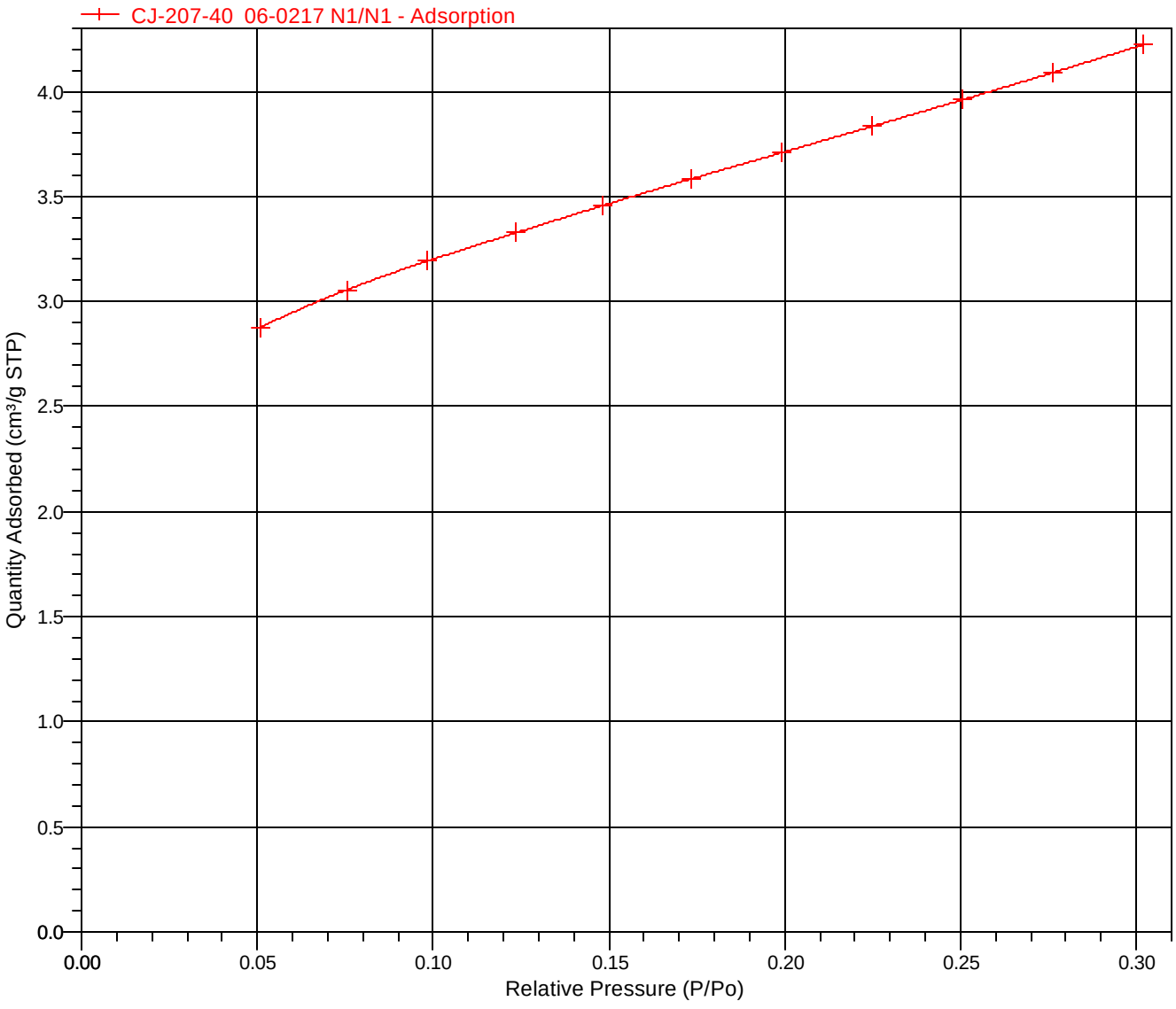
Relative Pressure (P/Po)	Absolute Pressure (mmHg)	Quantity Adsorbed (cm³/g STP)	Elapsed Time (h:min)	Saturation Pressure (mmHg)
			01:08	736.94562
0.051121487	37.68829	2.8779	02:10	
0.075556860	55.71075	3.0562	02:33	
0.098313891	72.49754	3.1924	02:49	
0.123338473	90.95711	3.3267	03:00	
			03:09	737.50061
0.148133515	109.24856	3.4562	03:09	
0.173619345	128.04437	3.5836	03:16	
0.199105163	146.84018	3.7082	03:23	
0.224676473	165.69904	3.8333	03:30	
0.250356073	184.63776	3.9600	03:37	
0.276132543	203.64792	4.0890	03:43	
0.302022993	222.74214	4.2212	03:49	

Sample: CJ-207-40 06-0217 N1/N1
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0217.SMP

Started:	2/1/2006 4:22:41PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 8:12:53PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/2/2006 7:50:36AM	Sample Mass:	4.3543 g
Warm Free Space:	5.5902 cm³ Measured	Cold Free Space:	15.9894 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Linear Plot



Sample: CJ-207-40 06-0217 N1/N1
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0217.SMP

Started: 2/1/2006 4:22:41PM
Completed: 2/1/2006 8:12:53PM
Report Time: 2/2/2006 7:50:36AM
Warm Free Space: 5.5902 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.3543 g
Cold Free Space: 15.9894 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Report

BET Surface Area: 13.1245 ± 0.0495 m²/g
Slope: 0.330055 ± 0.001233 g/cm³ STP
Y-Intercept: 0.001631 ± 0.000219 g/cm³ STP
C: 203.384811
Qm: 3.0149 cm³/g STP
Correlation Coefficient: 0.9999442
Molecular Cross-Sectional Area: 0.1620 nm²

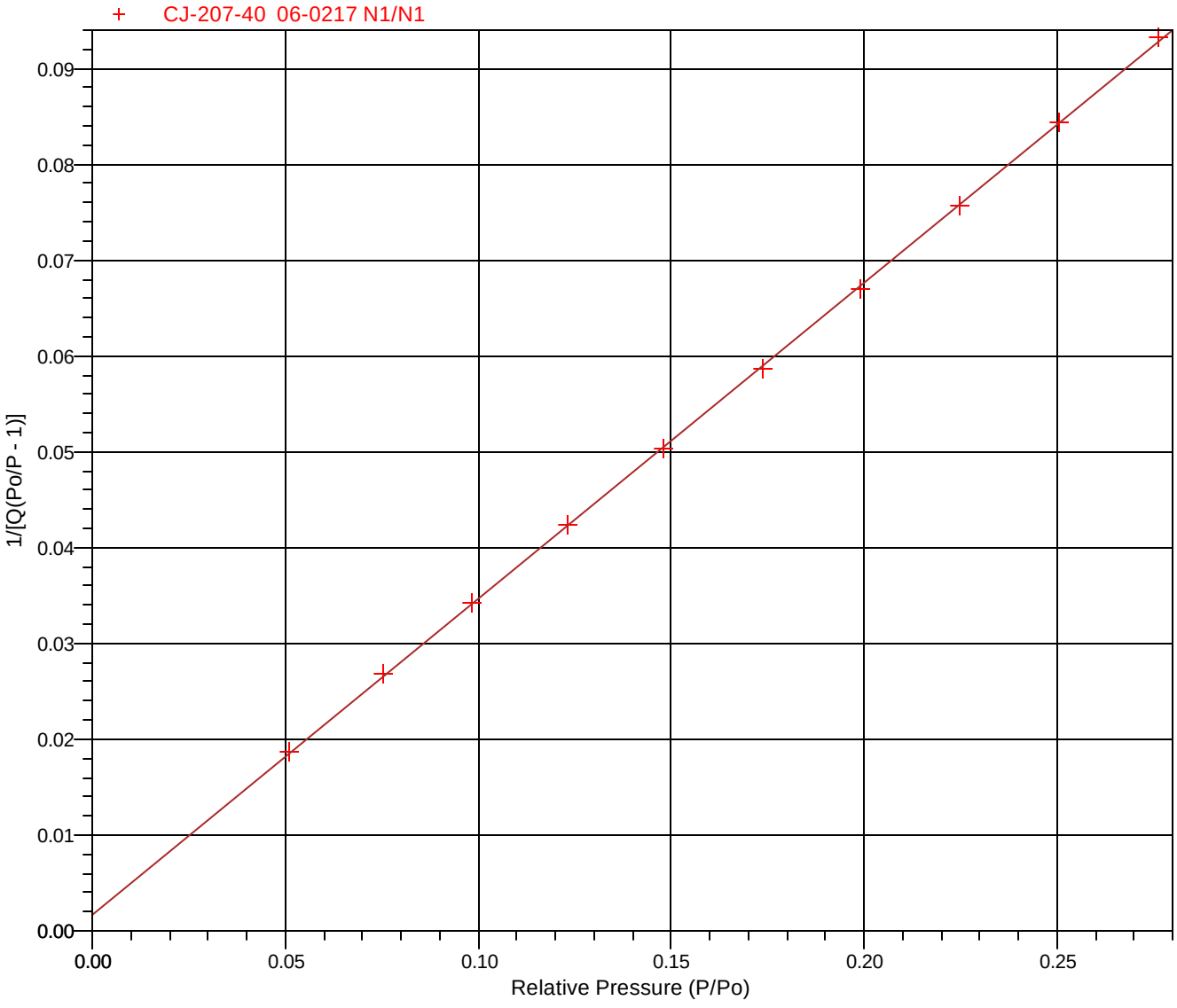
Relative Pressure (P/Po)	Quantity Adsorbed (cm³/g STP)	1/[Q(Po/P - 1)]
0.051121487	2.8779	0.018721
0.075556860	3.0562	0.026743
0.098313891	3.1924	0.034154
0.123338473	3.3267	0.042292
0.148133515	3.4562	0.050313
0.173619345	3.5836	0.058627
0.199105163	3.7082	0.067041
0.224676473	3.8333	0.075597
0.250356073	3.9600	0.084335
0.276132543	4.0890	0.093290

Sample: CJ-207-40 06-0217 N1/N1
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0217.SMP

Started:	2/1/2006 4:22:41PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 8:12:53PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/2/2006 7:50:36AM	Sample Mass:	4.3543 g
Warm Free Space:	5.5902 cm³ Measured	Cold Free Space:	15.9894 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Plot



Sample: CJ-207-40 06-0217 N1/N1
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0217.SMP

Started:	2/1/2006 4:22:41PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 8:12:53PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/2/2006 7:50:36AM	Sample Mass:	4.3543 g
Warm Free Space:	5.5902 cm³ Measured	Cold Free Space:	15.9894 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Summary Report

Surface Area

Single point surface area at P/Po = 0.276132543: 12.8851 m²/g

BET Surface Area: 13.1245 m²/g

Sample: CJ-208-40 06-0218 N2/N2
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0218.SMP

Started: 2/1/2006 4:22:41PM
Completed: 2/1/2006 8:12:53PM
Report Time: 2/1/2006 8:12:55PM
Warm Free Space: 5.7202 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.3662 g
Cold Free Space: 16.4086 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Tabular Report

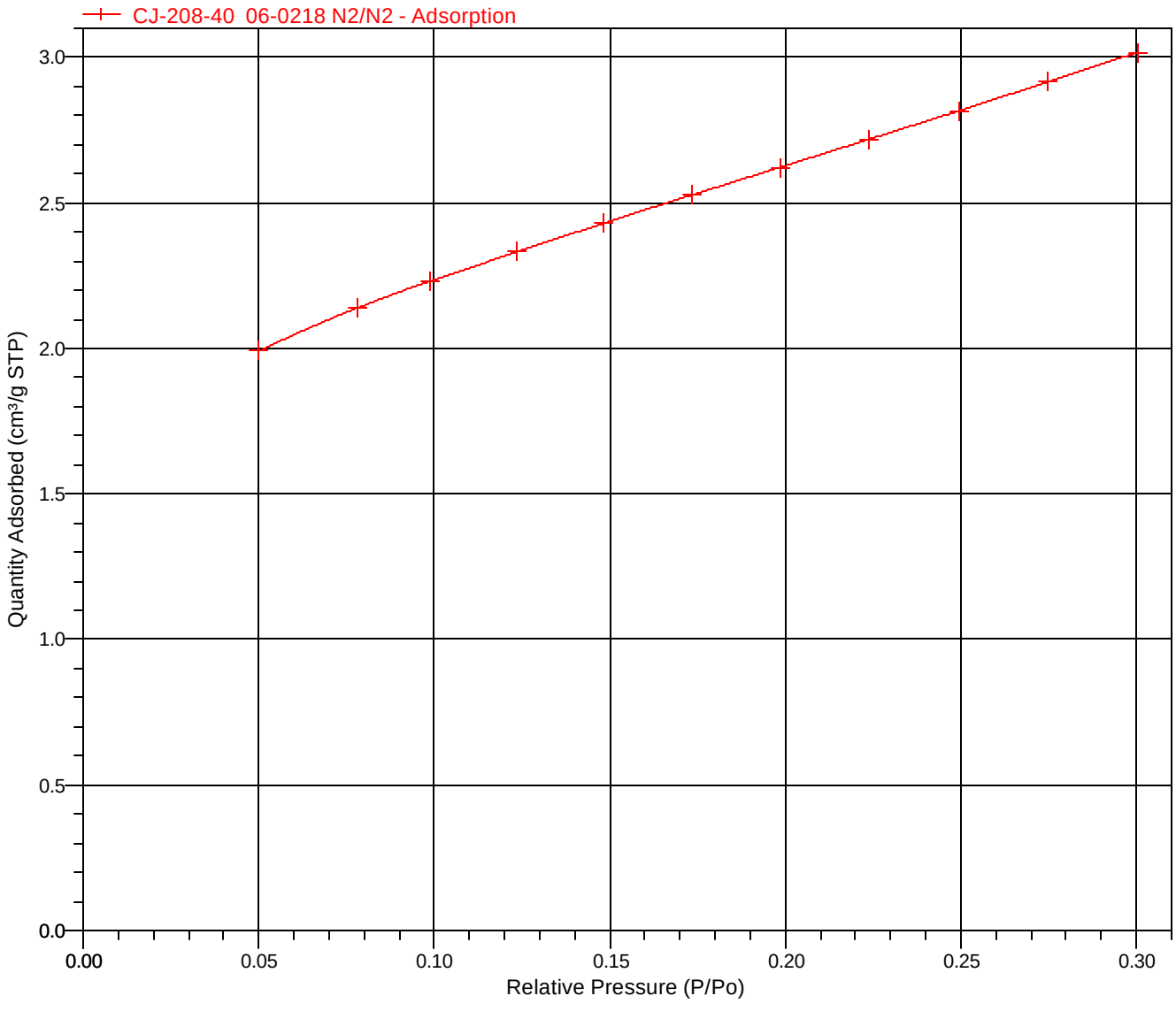
Relative Pressure (P/Po)	Absolute Pressure (mmHg)	Quantity Adsorbed (cm³/g STP)	Elapsed Time (h:min)	Saturation Pressure (mmHg)
			01:08	736.94562
0.050132413	36.94486	1.9911	01:38	
0.078159955	57.59964	2.1391	01:47	
0.098735843	72.76295	2.2310	01:57	
0.123546271	91.04688	2.3313	02:03	
0.148265749	109.26379	2.4301	02:08	
0.173383114	127.77393	2.5273	02:13	
0.198727824	146.45160	2.6228	02:18	
0.224004352	165.07903	2.7188	02:24	
0.249400225	183.79440	2.8166	02:28	
0.274898405	202.58517	2.9161	02:33	
0.300589849	221.51837	3.0177	02:38	

Sample: CJ-208-40 06-0218 N2/N2
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0218.SMP

Started:	2/1/2006 4:22:41PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 8:12:53PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 8:12:55PM	Sample Mass:	4.3662 g
Warm Free Space:	5.7202 cm³ Measured	Cold Free Space:	16.4086 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Linear Plot



Sample: CJ-208-40 06-0218 N2/N2
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0218.SMP

Started: 2/1/2006 4:22:41PM
Completed: 2/1/2006 8:12:53PM
Report Time: 2/1/2006 8:12:55PM
Warm Free Space: 5.7202 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.3662 g
Cold Free Space: 16.4086 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Report

BET Surface Area: 9.3897 ± 0.0250 m²/g
Slope: 0.460156 ± 0.001212 g/cm³ STP
Y-Intercept: 0.003458 ± 0.000232 g/cm³ STP
C: 134.056409
Qm: 2.1570 cm³/g STP
Correlation Coefficient: 0.9999688
Molecular Cross-Sectional Area: 0.1620 nm²

Relative Pressure (P/Po)	Quantity Adsorbed (cm³/g STP)	1/[Q(Po/P - 1)]
0.050132413	1.9911	0.026507
0.078159955	2.1391	0.039637
0.098735843	2.2310	0.049105
0.123546271	2.3313	0.060466
0.148265749	2.4301	0.071634
0.173383114	2.5273	0.082995
0.198727824	2.6228	0.094562
0.224004352	2.7188	0.106174
0.249400225	2.8166	0.117966
0.274898405	2.9161	0.130006
0.300589849	3.0177	0.142417

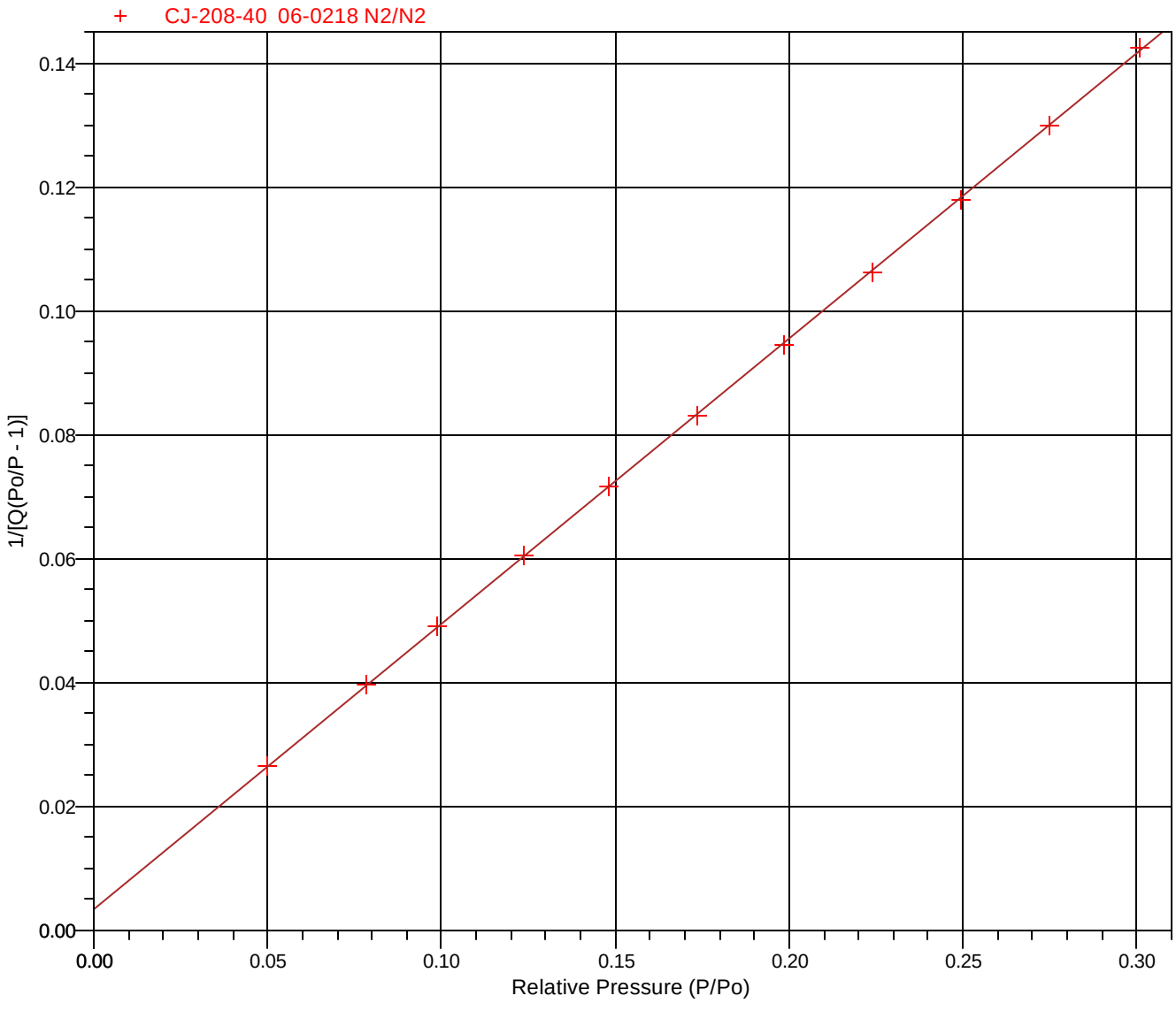
Sample: CJ-208-40 06-0218 N2/N2
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0218.SMP

Started: 2/1/2006 4:22:41PM
Completed: 2/1/2006 8:12:53PM
Report Time: 2/1/2006 8:12:55PM
Warm Free Space: 5.7202 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 4.3662 g
Cold Free Space: 16.4086 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Plot



Sample: CJ-208-40 06-0218 N2/N2
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0218.SMP

Started:	2/1/2006 4:22:41PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 8:12:53PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 8:12:55PM	Sample Mass:	4.3662 g
Warm Free Space:	5.7202 cm³ Measured	Cold Free Space:	16.4086 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Summary Report

Surface Area

Single point surface area at P/Po = 0.300589849: 9.1880 m²/g

BET Surface Area: 9.3897 m²/g

Sample: CJ-209-40 06-0219 N5/N5
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0219.SMP

Started: 2/1/2006 4:23:29PM
Completed: 2/1/2006 7:40:08PM
Report Time: 2/1/2006 7:40:06PM
Warm Free Space: 5.4357 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 5.1155 g
Cold Free Space: 15.2828 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Tabular Report

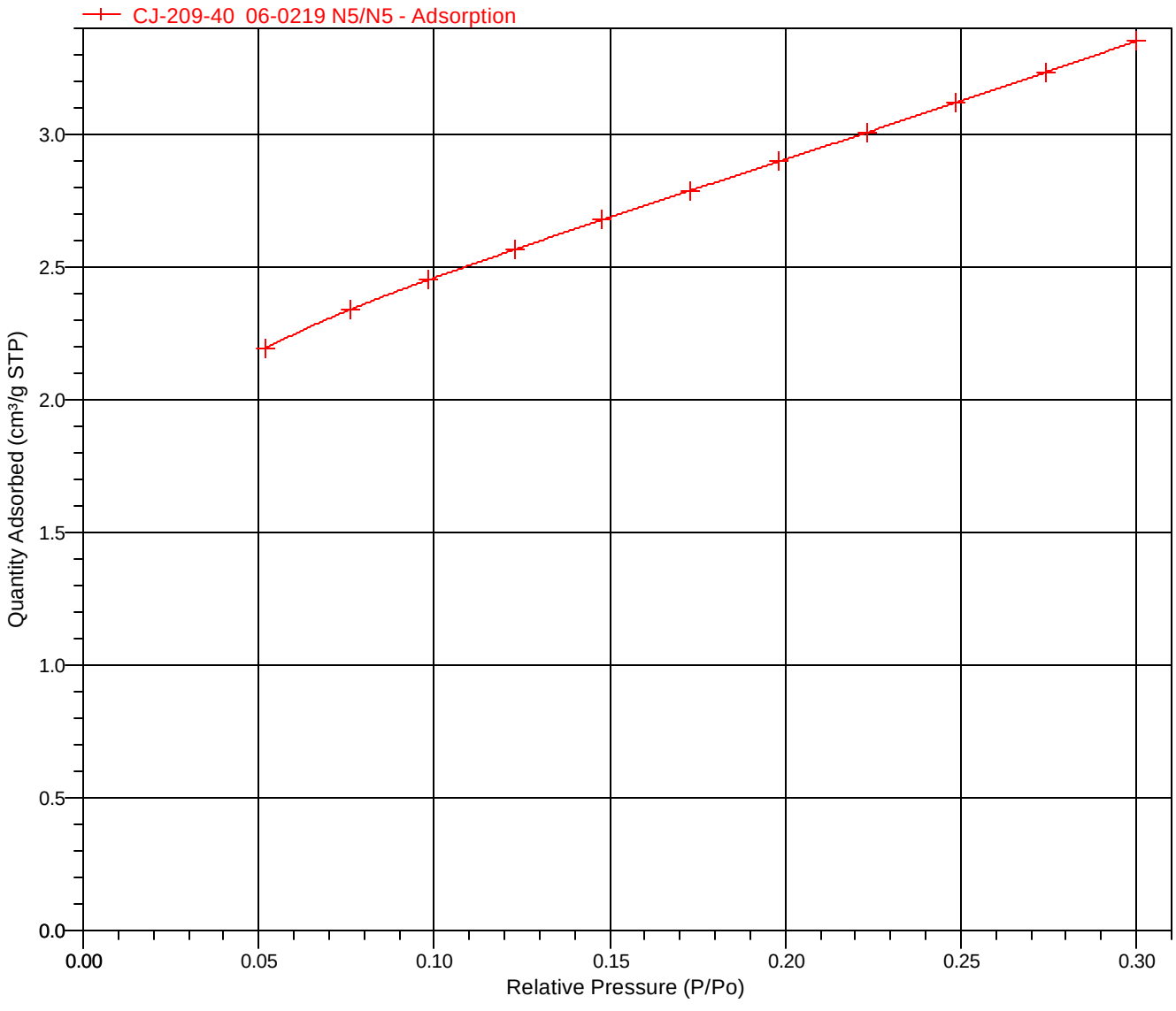
Relative Pressure (P/Po)	Absolute Pressure (mmHg)	Quantity Adsorbed (cm³/g STP)	Elapsed Time (h:min)	Saturation Pressure (mmHg)
			01:10	736.09106
0.051788686	38.12119	2.1947	01:36	
0.076204501	56.09345	2.3405	01:47	
0.098370893	72.40993	2.4519	01:55	
0.122832732	90.41608	2.5662	02:03	
0.147622492	108.66360	2.6782	02:09	
0.172751686	127.16097	2.7882	02:15	
0.197898138	145.67105	2.8976	02:21	
0.223314975	164.38016	3.0077	02:27	
0.248559218	182.96222	3.1200	02:32	
0.274240708	201.86613	3.2344	02:37	
0.300100534	220.90132	3.3510	02:42	

Sample: CJ-209-40 06-0219 N5/N5
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0219.SMP

Started:	2/1/2006 4:23:29PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 7:40:08PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 7:40:06PM	Sample Mass:	5.1155 g
Warm Free Space:	5.4357 cm³ Measured	Cold Free Space:	15.2828 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Linear Plot



Sample: CJ-209-40 06-0219 N5/N5
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0219.SMP

Started: 2/1/2006 4:23:29PM
Completed: 2/1/2006 7:40:08PM
Report Time: 2/1/2006 7:40:06PM
Warm Free Space: 5.4357 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 5.1155 g
Cold Free Space: 15.2828 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Report

BET Surface Area: 10.4560 ± 0.0226 m²/g
Slope: 0.412643 ± 0.000883 g/cm³ STP
Y-Intercept: 0.003694 ± 0.000169 g/cm³ STP
C: 112.707884
Qm: 2.4019 cm³/g STP
Correlation Coefficient: 0.9999794
Molecular Cross-Sectional Area: 0.1620 nm²

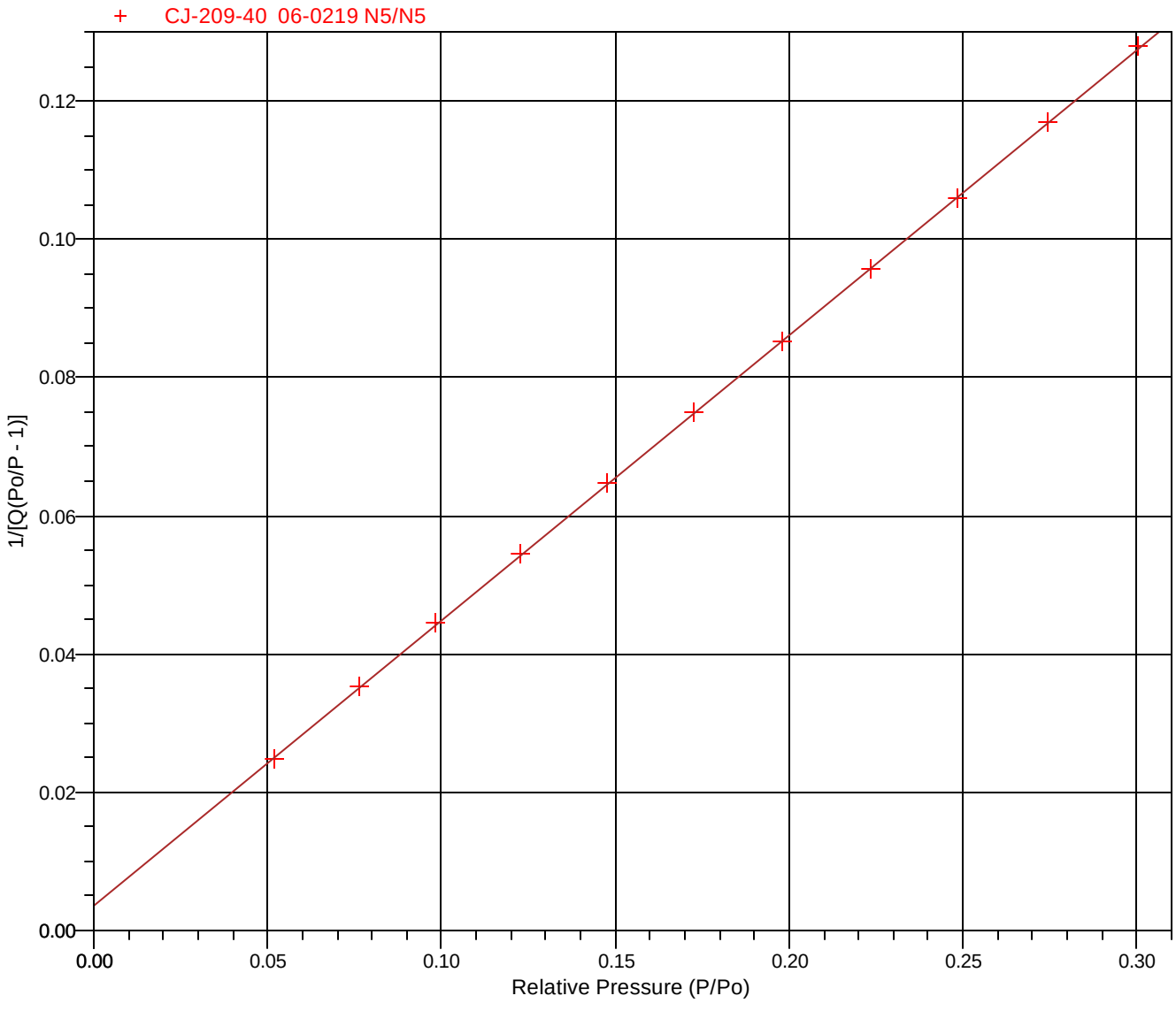
Relative Pressure (P/Po)	Quantity Adsorbed (cm³/g STP)	1/[Q(Po/P - 1)]
0.051788686	2.1947	0.024886
0.076204501	2.3405	0.035244
0.098370893	2.4519	0.044498
0.122832732	2.5662	0.054568
0.147622492	2.6782	0.064665
0.172751686	2.7882	0.074897
0.197898138	2.8976	0.085148
0.223314975	3.0077	0.095596
0.248559218	3.1200	0.106018
0.274240708	3.2344	0.116828
0.300100534	3.3510	0.127954

Sample: CJ-209-40 06-0219 N5/N5
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0219.SMP

Started:	2/1/2006 4:23:29PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 7:40:08PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/1/2006 7:40:06PM	Sample Mass:	5.1155 g
Warm Free Space:	5.4357 cm³ Measured	Cold Free Space:	15.2828 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Plot



Sample: CJ-209-40 06-0219 N5/N5
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0219.SMP

Started: 2/1/2006 4:23:29PM
Completed: 2/1/2006 7:40:08PM
Report Time: 2/1/2006 7:40:06PM
Warm Free Space: 5.4357 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 5.1155 g
Cold Free Space: 15.2828 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Summary Report

Surface Area

Single point surface area at P/Po = 0.300100534: 10.2099 m²/g

BET Surface Area: 10.4560 m²/g

Sample: CJ-210-40 06-0220 N6/N6
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0220.SMP

Started: 2/1/2006 4:23:29PM
Completed: 2/1/2006 7:40:08PM
Report Time: 2/2/2006 7:51:21AM
Warm Free Space: 5.6495 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 5.1428 g
Cold Free Space: 16.1759 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Tabular Report

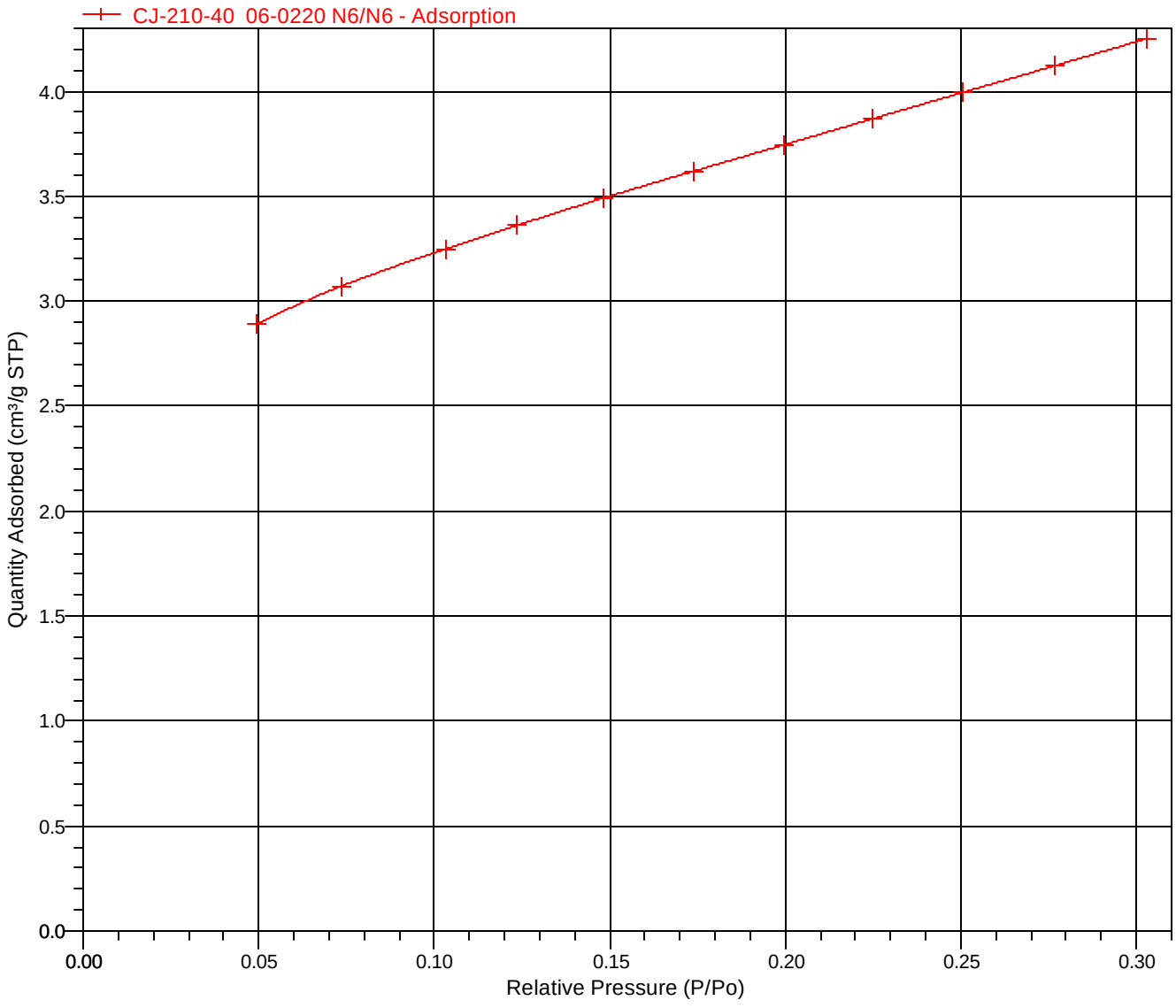
Relative Pressure (P/Po)	Absolute Pressure (mmHg)	Quantity Adsorbed (cm³/g STP)	Elapsed Time (h:min)	Saturation Pressure (mmHg)
			01:10	736.09106
0.049305304	36.29458	2.8912	01:51	
0.073760837	54.29753	3.0722	02:06	
0.103302563	76.04499	3.2499	02:19	
0.123540210	90.94355	3.3609	02:29	
0.148244880	109.13059	3.4916	02:37	
0.173779264	127.92847	3.6198	02:43	
0.199364321	146.76399	3.7447	02:50	
0.224954724	165.60370	3.8690	02:57	
0.250692811	184.55220	3.9948	03:03	
0.276623808	203.64293	4.1218	03:09	
			03:11	736.17419
0.302748904	222.87593	4.2511	03:15	

Sample: CJ-210-40 06-0220 N6/N6
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0220.SMP

Started:	2/1/2006 4:23:29PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 7:40:08PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/2/2006 7:51:21AM	Sample Mass:	5.1428 g
Warm Free Space:	5.6495 cm³ Measured	Cold Free Space:	16.1759 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Isotherm Linear Plot



Sample: CJ-210-40 06-0220 N6/N6
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0220.SMP

Started: 2/1/2006 4:23:29PM
Completed: 2/1/2006 7:40:08PM
Report Time: 2/2/2006 7:51:21AM
Warm Free Space: 5.6495 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 5.1428 g
Cold Free Space: 16.1759 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Report

BET Surface Area: 13.2247 ± 0.0591 m²/g
Slope: 0.327644 ± 0.001449 g/cm³ STP
Y-Intercept: 0.001529 ± 0.000258 g/cm³ STP
C: 215.310851
Qm: 3.0379 cm³/g STP
Correlation Coefficient: 0.9999217
Molecular Cross-Sectional Area: 0.1620 nm²

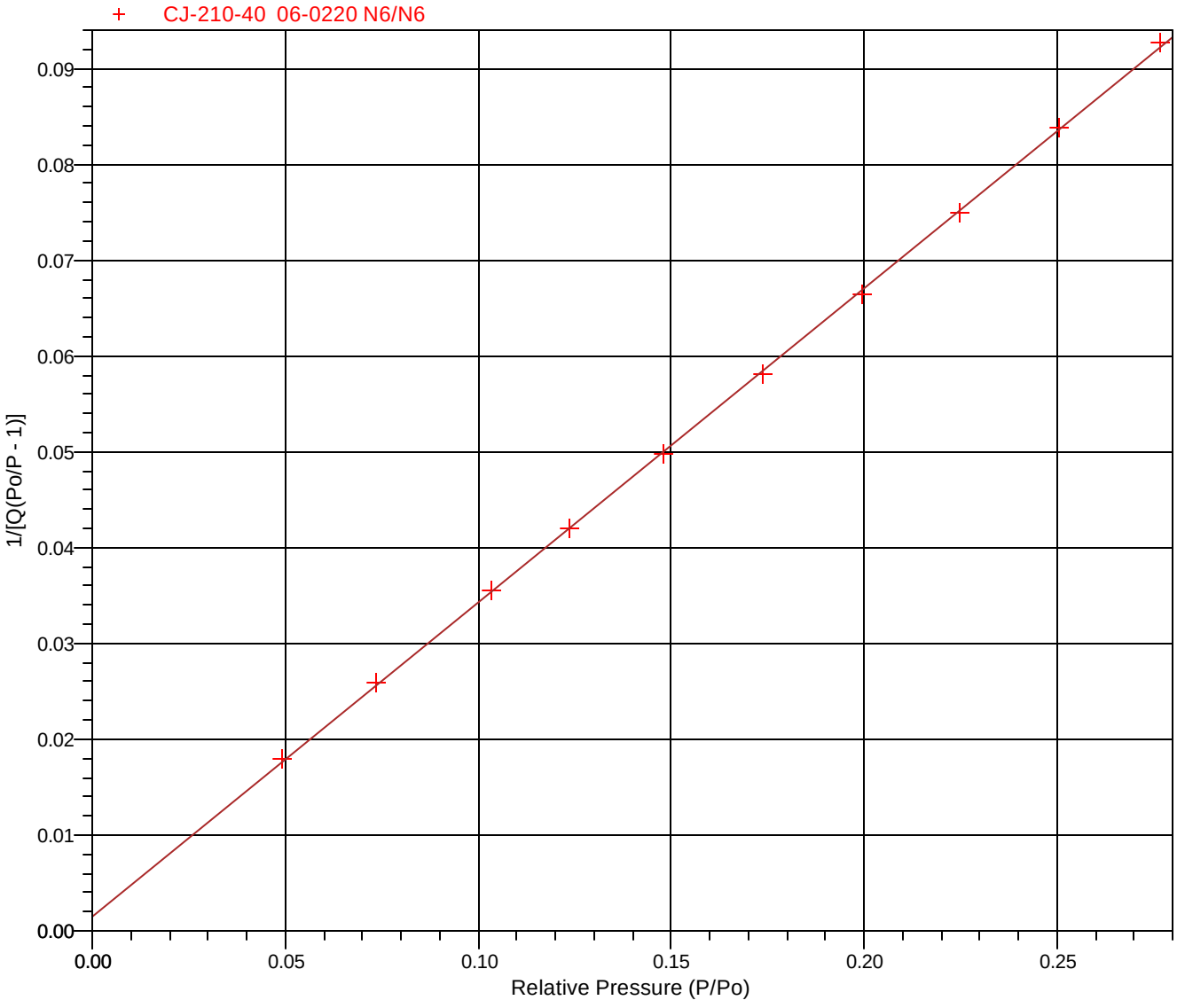
Relative Pressure (P/Po)	Quantity Adsorbed (cm³/g STP)	1/[Q(Po/P - 1)]
0.049305304	2.8912	0.017938
0.073760837	3.0722	0.025921
0.103302563	3.2499	0.035448
0.123540210	3.3609	0.041939
0.148244880	3.4916	0.049847
0.173779264	3.6198	0.058106
0.199364321	3.7447	0.066495
0.224954724	3.8690	0.075018
0.250692811	3.9948	0.083751
0.276623808	4.1218	0.092777

Sample: CJ-210-40 06-0220 N6/N6
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0220.SMP

Started:	2/1/2006 4:23:29PM	Analysis Adsorptive:	N2
Completed:	2/1/2006 7:40:08PM	Analysis Bath Temp.:	77.300 K
Report Time:	2/2/2006 7:51:21AM	Sample Mass:	5.1428 g
Warm Free Space:	5.6495 cm³ Measured	Cold Free Space:	16.1759 cm³ Measured
Equilibration Interval:	10 s	Low Pressure Dose:	None
Sample Density:	1.000 g/cm³	Automatic Degas:	Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

BET Surface Area Plot



Sample: CJ-210-40 06-0220 N6/N6
Operator: MJP
Submitter: S.M.Stoller
File: C:\...\01JAN\06-0220.SMP

Started: 2/1/2006 4:23:29PM
Completed: 2/1/2006 7:40:08PM
Report Time: 2/2/2006 7:51:21AM
Warm Free Space: 5.6495 cm³ Measured
Equilibration Interval: 10 s
Sample Density: 1.000 g/cm³

Analysis Adsorptive: N2
Analysis Bath Temp.: 77.300 K
Sample Mass: 5.1428 g
Cold Free Space: 16.1759 cm³ Measured
Low Pressure Dose: None
Automatic Degas: Yes

Sample Prep: Stage	Soak Temperature (°C)	Ramp Rate (°C/min)	Soak Time (min)
1	100	10	960

Summary Report

Surface Area

Single point surface area at P/Po = 0.276623808: 12.9795 m²/g

BET Surface Area: 13.2247 m²/g

Appendix F

PHREEQC Input Files for Sequential Batch Reaction Models

List of Files

(1) Transport_seq_batch_horizontal
(2) Transport_seq_batch_vertical

```
TITLE Crescent Junction Transport Model - Horizontal Transport in Sequential Batch
Test
# Includes Mineral PPT, adsorption, and IX
# Transport of Tailings Water through Mancos Shale
# Database "Phreeqc_Davis_Naturita_GC_Short.txt"
# GC (Generalized Composite) Adsorption Model (to match Davis and Curtis Figure 5.6)
# React in 3 separate batch steps using "fresh" Mancos (from 40-ft depth) each step
# Use BH210 gw only to set the IX and adsorption sites
# Added U to BH210 to get the right amount adsorbed to show the measured U increase
SOLUTION 0  SPF-1 (Tailings Fluid). Using final control values from batch tests.
     temp       25
        pH      7.85
        pe      7
        redox   pe
        units   mg/L
        Alkalinity      510.0 as CaCO3
        Amm     2000
        Ca      196
        Na      5300
        Mg      310
        K       129
        S(6)    18272   as SO4
        Cl      1018
SOLUTION 1  Groundwater from CJ BH 210. Initial solution for exchange sites
# Groundwater chemistry from Borehole 210 (CJ)
#   sampled 11/7/05. This sample is considered represenative of Mancos groundwater
# This composition sets the initial conditions for the exchange sites
        units            mg/L
        temp             25.0
        pH               7.23
        pe               12.5
        Alkalinity      634 as CaCO3
#       Amm              0
        Ca              180
        Na              12000
        Mg              140
        K               58
        S(6)            1700 as SO4
        Cl              23000
        U                       0.2
END

EXCHANGE 1
        equilibrate  with solution 1
# Used 400 mL fluid with 100g rock, ie. R/W = 250g/L
# Mean measured CEC=11.23 meq/L
# Exchange Sites = 250 g/L x 11.23 meq/100g x 1 eq/1000 meq = 0.028 eq/L
               X                        0.028
SURFACE 1
# Site Density =  (1.92 umoles hydroxyl sites)/m^2 (assumed bidentate bonds)
#       from Davis and Kent (1990) and
#       used in Davis and Curtis (2003) Naturita GC Model
# Surface area (Mean of 10 values from 1-2 mm fraction) = 11.02 m^2/g (BET
Measurement)
# Used 250 g rock/L gw
# Of Total Sites: Very Strong Sites = 0.01 %, Strong Sites = 1.2 % (Davis and
Curtis)
# Total Sites = 5290 umol sites/L gw  (from 250*11.02*1.92)
# Very Strong Sites = 0.0001*5290 = 0.53 umoles/L (5.3e-7 mol/L)
# Strong Sites = 0.012 * 5290 = 63.5 umoles/L  (6.35e-5 mol/L)
# Weak Sites = 0.9879 * 5290 = 5226 umoles/L  (5.226e-3 mol/L)
        -equilibrate with solution 1
        Hfo_wOH         5.226e-3        11.02     250.0
```

```
        Hfo_sOH         6.35e-5 11.02     250.0
        Hfo_vOH         5.3e-7  11.02     250.0
        -no_edl
End

Use Solution 0
Use Exchange 1
Use Surface 1
Equilibrium_Phases 1
# The total no. of moles is based on water soluble and XRD tests of Mancos Shale
# For verticle transport through deeper Mancos (in mol/Lgw):Gypsum 6.67e-4,
Nahcolite 0.017
# For horizontal transport through shallower Mancos (in mol/Lgw):Gypsum 0.017,
Nahcolite 6.67e-3
# Calcite 1 wgt % = 0.025 mol/Lgw for all depths. Calcite was not completely
dissolved in tests.
# Halite 6.67e-4 mol/Lgw for all depths
        Calcite 0.0     0.025
        Gypsum  0.0     0.017
        Nahcolite       0.0     6.67e-3
        Halite  0.0     6.67e-4

PRINT
        -reset          true
SELECTED_OUTPUT
        -file            transport_seq_batch_horizontal.sel
        -totals          Na Amm K Ca Cl U S(6)
        -molalities              NaX AmmHX KX CaX2
Save Solution 0
END
Use Solution 0
Use Exchange 1
Use Surface 1
Equilibrium_Phases 1
# The total no. of moles is based on water soluble and XRD tests of Mancos Shale
# For verticle transport through deeper Mancos (in mol/Lgw):Gypsum 6.67e-4,
Nahcolite 0.017
# For horizontal transport through shallower Mancos (in mol/Lgw):Gypsum 0.017,
Nahcolite 6.67e-3
# Calcite 1 wgt % = 0.025 mol/Lgw for all depths. Calcite was not completely
dissolved in tests.
# Halite 6.67e-4 mol/Lgw for all depths
        Calcite 0.0     0.025
        Gypsum  0.0     0.017
        Nahcolite       0.0     6.67e-3
        Halite  0.0     6.67e-4

PRINT
        -reset          true
SELECTED_OUTPUT
        -file            transport_seq_batch_horizontal.sel
        -totals          Na Amm K Ca Cl U S(6)
        -molalities              NaX AmmHX KX CaX2
Save Solution 0
END
Use Solution 0
Use Exchange 1
Use Surface 1
Equilibrium_Phases 1
# The total no. of moles is based on water soluble and XRD tests of Mancos Shale
# For verticle transport through deeper Mancos (in mol/Lgw):Gypsum 6.67e-4,
Nahcolite 0.017
# For horizontal transport through shallower Mancos (in mol/Lgw):Gypsum 0.017,
```

```
Nahcolite 6.67e-3
# Calcite 1 wgt % = 0.025 mol/Lgw for all depths. Calcite was not completely
dissolved in tests.
# Halite 6.67e-4 mol/Lgw for all depths
        Calcite 0.0     0.025
        Gypsum  0.0     0.017
        Nahcolite       0.0     6.67e-3
        Halite  0.0     6.67e-4

PRINT
        -reset          true
SELECTED_OUTPUT
        -file            transport_seq_batch_horizontal.sel
        -totals          Na Amm K Ca Cl U S(6)
        -molalities              NaX AmmHX KX CaX2
END
```

```
TITLE Crescent Junction Transport Model - Verticle Transport in Sequential Batch
Test
# Includes Mineral PPT, adsorption, and IX
# Transport of Tailings Water through Mancos Shale
# Database "Phreeqc_Davis_Naturita_GC_Short.txt"
# GC (Generalized Composite) Adsorption Model (to match Davis and Curtis Figure 5.6)
# React in 5 separate batch steps using "fresh" Mancos (from 40-ft depth) at first
step
#       then, "fresh" Mancos from deeper (lower gypsum) for remaining steps
# Use BH210 gw only to set the IX and adsorption sites
# Added U to BH210 to get the right amount adsorbed to show the measured U increase
SOLUTION 0  SPF-1 (Tailings Fluid). Using final control values from batch tests.
     temp       25
        pH      6.63
        pe      7
        redox   pe
        units   mg/L
        Alkalinity      510.0 as CaCO3
        Amm     2000
        Ca      196
        Na      5300
        Mg      310
        K       129
        S(6)    18272   as SO4
        Cl      1018
SOLUTION 1  Groundwater from CJ BH 210. Initial solution for exchange sites
# Groundwater chemistry from Borehole 210 (CJ)
#   sampled 11/7/05. This sample is considered represenative of Mancos groundwater
# This composition sets the initial conditions for the exchange sites
        units            mg/L
        temp             25.0
        pH               7.23
        pe               12.5
        Alkalinity      634 as CaCO3
#       Amm              0
        Ca              180
        Na              12000
        Mg              140
        K               58
        S(6)            1700 as SO4
        Cl              23000
        U               0.2
END

EXCHANGE 1
        equilibrate  with solution 1
# Used 400 mL fluid with 100g rock, ie. R/W = 250g/L
# Mean measured CEC=11.23 meq/L
# Exchange Sites = 250 g/L x 11.23 meq/100g x 1 eq/1000 meq = 0.028 eq/L
                X                       0.028
SURFACE 1
# Site Density =  (1.92 umoles hydroxyl sites)/m^2 (assumed bidentate bonds)
#       from Davis and Kent (1990) and
#       used in Davis and Curtis (2003) Naturita GC Model
# Surface area (Mean of 10 values from 1-2 mm fraction) = 11.02 m^2/g (BET
Measurement)
# Used 250 g rock/L gw
# Of Total Sites: Very Strong Sites = 0.01 %, Strong Sites = 1.2 % (Davis and
Curtis)
# Total Sites = 5290 umol sites/L gw  (from 250*11.02*1.92)
# Very Strong Sites = 0.0001*5290 = 0.53 umoles/L (5.3e-7 mol/L)
# Strong Sites = 0.012 * 5290 = 63.5 umoles/L  (6.35e-5 mol/L)
# Weak Sites = 0.9879 * 5290 = 5226 umoles/L  (5.226e-3 mol/L)
```

```
        -equilibrate with solution 1
        Hfo_wOH         5.226e-3        11.02     250.0
        Hfo_sOH         6.35e-5         11.02     250.0
        Hfo_vOH         5.3e-7          11.02     250.0
        -no_edl
End

# Reaction with 40-ft depth sample
Use Solution 0
Use Exchange 1
Use Surface 1
#PHASES
#       Fix_H+
#       H+ = H+
#       log_k  0.0
Equilibrium_Phases 1
# The total no. of moles is based on water soluble and XRD tests of Mancos Shale
# For verticle transport through deeper Mancos (in mol/Lgw):Gypsum 6.67e-4,
Nahcolite 0.017
# For horizontal transport through shallower Mancos (in mol/Lgw):Gypsum 0.017,
Nahcolite 6.67e-3
# Calcite 1 wgt % = 0.025 mol/Lgw for all depths. Calcite was not completely
dissolved in tests.
# Halite 6.67e-4 mol/Lgw for all depths
        Calcite         0.0     0.025
        Gypsum          0.0     0.01
        Nahcolite       0.0     6.67e-3
        Halite          0.0     6.67e-4
#       CO2(g)  -2.1    1.0
#     Fix_H+            -7.73   CO2(g)    10.0
PRINT
        -reset          true
Save Solution 0
END

# Reaction with 105-ft depth sample
Use Solution 0
Use Exchange 1
Use Surface 1
Equilibrium_Phases 1
# The total no. of moles is based on water soluble and XRD tests of Mancos Shale
# For verticle transport through deeper Mancos (in mol/Lgw):Gypsum 6.67e-4,
Nahcolite 0.017
# For horizontal transport through shallower Mancos (in mol/Lgw):Gypsum 0.017,
Nahcolite 6.67e-3
# Calcite 1 wgt % = 0.025 mol/Lgw for all depths. Calcite was not completely
dissolved in tests.
# Halite 6.67e-4 mol/Lgw for all depths
        Calcite         0.0     0.025
        Gypsum          0.0     6.67e-4
        Nahcolite       0.0     0.017
        Halite          0.0     6.67e-4
PRINT
        -reset          true
Save Solution 0
END

# Reaction with 170-ft sample
Use Solution 0
Use Exchange 1
Use Surface 1
Equilibrium_Phases 1
# The total no. of moles is based on water soluble and XRD tests of Mancos Shale
```

```
# For verticle transport through deeper Mancos (in mol/Lgw):Gypsum 6.67e-4,
Nahcolite 0.017
# For horizontal transport through shallower Mancos (in mol/Lgw):Gypsum 0.017,
Nahcolite 6.67e-3
# Calcite 1 wgt % = 0.025 mol/Lgw for all depths. Calcite was not completely
dissolved in tests.
# Halite 6.67e-4 mol/Lgw for all depths
        Calcite         0.0     0.025
        Gypsum          0.0     6.67e-4
        Nahcolite       0.0     0.017
        Halite          0.0     6.67e-4
PRINT
        -reset          true
Save Solution 0
END

# Reaction with 235-ft sample
Use Solution 0
Use Exchange 1
Use Surface 1
Equilibrium_Phases 1
# The total no. of moles is based on water soluble and XRD tests of Mancos Shale
# For verticle transport through deeper Mancos (in mol/Lgw):Gypsum 6.67e-4,
Nahcolite 0.017
# For horizontal transport through shallower Mancos (in mol/Lgw):Gypsum 0.017,
Nahcolite 6.67e-3
# Calcite 1 wgt % = 0.025 mol/Lgw for all depths. Calcite was not completely
dissolved in tests.
# Halite 6.67e-4 mol/Lgw for all depths
        Calcite         0.0     0.025
        Gypsum          0.0     6.67e-4
        Nahcolite       0.0     0.017
        Halite          0.0     6.67e-4
PRINT
        -reset          true
Save Solution 0
END

# Reaction with 300-ft sample
Use Solution 0
Use Exchange 1
Use Surface 1
Equilibrium_Phases 1
# The total no. of moles is based on water soluble and XRD tests of Mancos Shale
# For verticle transport through deeper Mancos (in mol/Lgw):Gypsum 6.67e-4,
Nahcolite 0.017
# For horizontal transport through shallower Mancos (in mol/Lgw):Gypsum 0.017,
Nahcolite 6.67e-3
# Calcite 1 wgt % = 0.025 mol/Lgw for all depths. Calcite was not completely
dissolved in tests.
# Halite 6.67e-4 mol/Lgw for all depths
        Calcite         0.0     0.025
        Gypsum          0.0     6.67e-4
        Nahcolite       0.0     0.017
        Halite          0.0     6.67e-4
PRINT
        -reset          true
Save Solution 0
END
```

Appendix G

PHREEQC Input Files for Transport Models

List of Files

(1) *Transport_horizontal*
(2) *Transport_vertical*

```
TITLE Crescent Junction Transport Model - Horizontal Transport Through Mancos Shale
# Includes Mineral PPT, adsorption, and IX
# Transport of Tailings Water through Mancos Shale
# Database "Phreeqc_Davis_Naturita_GC_Short.txt"
# GC (Generalized Composite) Adsorption Model (to match Davis and Curtis Figure 5.6)
#
#
SOLUTION 0  SPF-1 (Tailings Fluid)
     temp       25
        pH      6.63
        pe      7
        redox   pe
        units   mg/L
        Alkalinity      570.0 as CaCO3
        Amm     2181.82
        Ca      209.62
        Na      5781.41
        Mg      315.71
        K       112.23
        S(6)    17454.37        as SO4
        Cl      910.26
        U       4.0
SOLUTION 1-40  Groundwater from CJ BH 210. Initial solution for column
# Groundwater chemistry from Borehole 210 (CJ)
#   sampled 11/7/05. This sample is considered representative of Mancos groundwater
        units           mg/L
        temp            25.0
        pH              7.23
        pe              12.5
        Alkalinity      634 as CaCO3
#       Amm             0
        Ca              180
        Na              12000
        Mg              140
        K               58
        S(6)            1700 as SO4
        Cl              23000
# Uranium concentration was calibrated by seq batch test model to produce
#       the amount of required adsorption. 0.2 /30 = 0.0067mg/L
        U                       0.0067
END

# Equilibrate BH 210 Fluid with Calcite and Gypsum
USE solution 1
Equilibrium_Phases
        Calcite 0.0     10.0
        Gypsum  0.0     10.0
Save solution 1
End
# Equilibrate Soln 1 (BH 210) with exchange sites and Minerals
EXCHANGE 1-20
        equilibrate  with solution 1
# R/W = 7500 g/L
# Mean measured CEC=11.23 meq/100g
# Exchange Sites = 7500 g/L x 11.23 meq/100g x 1 eq/1000 meq = 0.842 eq/L
                X                               0.842
Equilibrium_Phases 1-20
# The total no. of moles is based on water soluble and XRD tests of Mancos Shale
# For verticle transport through deeper Mancos (in mol/Lgw):Gypsum 0.02, Nahcolite
0.5
# For horizontal transport through shallower Mancos (in mol/Lgw):Gypsum 0.5,
Nahcolite 0.2
# Calcite 1 wgt % = 0.75 mol/Lgw for all depths. Calcite was not completely
```

```
dissolved in tests.
# Halite 0.02 mol/Lgw for all depths
        Calcite         0.0     0.75
        Gypsum          0.0     0.5
        Nahcolite       0.0     0.2
        Halite          0.0     0.02
SURFACE 1-20
# Site Density =  (1.92 umoles hydroxyl sites)/m^2 (assumed bidentate bonds)
#       from Davis and Kent (1990) and
#       used in Davis and Curtis (2003) Naturita GC Model
# Surface area (Mean of 10 values from 1-2 mm fraction) = 11.02 m^2/g (BET
Measurement)
# Used 7500 g rock/Lgw
# Of Total Sites: Very Strong Sites = 0.01 %, Strong Sites = 1.2 % (Davis and
Curtis)
# Total Sites = 158,688 umol sites/L gw  (from 7500*11.02*1.92)
# Very Strong Sites = 0.0001*158688 = 15.87 umoles/L (SJM Calculation)
# Strong Sites = 0.012 * 158688 = 1904 umoles/L  (SJM Calculation)
# Weak Sites = 0.9879 * 158688 = 156768 umoles/L  (SJM Calculation)
        -equilibrate 1
        Hfo_wOH         1.568e-1        11.02   7500.0
        Hfo_sOH         1.904e-3        11.02   7500.0
        Hfo_vOH         1.587e-5        11.02   7500.0
        -no_edl
PRINT
        -reset          true
ADVECTION
        -cells           20
        -shifts          200
        -punch           20
#        -punch           10 20
        -punch_frequency 1
        -print           20
        -print_frequency 50
USER_GRAPH
        -headings PV Na C NH4*5 Ca*10 Cl SO4 U*1000 KD*25000 pH*1000
#       -headings PV TOTADS CS TOT("U") KD
        -chart_title "Crescent Junction Horizontal Transport Model"
        -axis_titles "PORE VOLUME" "Effluent Concentration (mg/L)"
        -axis_scale x_axis 0 10 1 0.1
        -axis_scale y_axis 0 25000.0 1000.0
        -initial_solutions false
        -plot_concentration_vs time
        -start
        5 TOTADS = MOL("Hfo_wOUO2OH") + MOL("Hfo_sOUO2CO3-") + MOL("Hfo_vOUO2OH") +
MOL("Hfo_vOUO2CO3-")
        6 CS = TOTADS/7500
        7 KD = (CS/TOT("U"))*1000
        10 GRAPH_X (STEP_NO + 0.5) / 20
        20 GRAPH_Y TOT("Na")*23000, TOT("C")*12000, TOT("Amm")*18000*5,
TOT("Ca")*40000*10, TOT("Cl")*35900, TOT("S(6)")*96000, TOT("U")*238000*1000,
KD*25000, 1000*(-LA"H+")
#       20 GRAPH_Y TOT("U")*238000*1000, KD*25000
        -end
PRINT
        -user_graph true
SELECTED_OUTPUT
        -file           CJ_transport.sel
        -totals         Na Amm K Ca Cl
        -molalities             NaX AmmHX KX CaX2
END
```

```
TITLE Crescent Junction Transport Model - Vertical Transport Through Mancos Shale
# Includes Mineral PPT, adsorption, and IX
# Transport of Tailings Water through Mancos Shale
# Database "Phreeqc_Davis_Naturita_GC_Short.txt"
# GC (Generalized Composite) Adsorption Model (to match Davis and Curtis Figure 5.6)
#
#
SOLUTION 0  SPF-1 (Tailings Fluid). From means in SOWP Table 9
     temp       25
        pH      6.63
        pe      7
        redox   pe
        units   mg/L
        Alkalinity      570.0 as CaCO3
        Amm     2181.82
        Ca      209.62
        Na      5781.41
        Mg      315.71
        K       112.23
        S(6)    17454.37        as SO4
        Cl      910.26
        U       4.0
SOLUTION 1-20  Groundwater from CJ BH 210. Initial solution for streamtube
# Groundwater chemistry from Borehole 210 (CJ)
#   sampled 11/7/05. This sample is considered represenative of Mancos groundwater
        units            mg/L
        temp             25.0
        pH               7.23
        pe               12.5
        Alkalinity      634 as CaCO3
#       Amm              0
        Ca              180
        Na              12000
        Mg              140
        K               58
        S(6)            1700 as SO4
        Cl              23000
# U value is 0.2 (used in model of Seq Batch) divided by 30 (W/R factor)
        U                       6.67e-3
END

# Equilibrate Tailings Fluid with Calcite
USE solution 0
PHASES
        Fix_H+
        H+ = H+
        log_k  0.0
Equilibrium_Phases
        Calcite 0.0     10.0
        Fix_H+   -6.63   NaOH    10.0
Save solution 0
End
# Equilibrate BH 210 Fluid with Calcite
USE solution 1
Equilibrium_Phases
        Calcite 0.0     10.0
        Fix_H+   -7.23   NaOH    10.0
#       Gypsum  0.0     10.0
Save solution 1
End
# Equilibrate Soln 1 (BH 210) with exchange sites and Minerals
EXCHANGE 1-20
        equilibrate  with solution 1
```

```
# R/W = 7500 g/L
# Mean measured CEC=11.23 meq/100g
# Exchange Sites = 7500 g/L x 11.23 meq/100g x 1 eq/1000 meq = 0.842 eq/L
                X                              0.842
Equilibrium_Phases 1-20
# The total no. of moles is based on water soluble and XRD tests of Mancos Shale
# For verticle transport through deeper Mancos (in mol/Lgw):Gypsum 0.02, Nahcolite
0.5
# For horizontal transport through shallower Mancos (in mol/Lgw):Gypsum 0.5,
Nahcolite 0.2
# Calcite 1 wgt % = 0.75 mol/Lgw for all depths. Calcite was not completely
dissolved in tests.
# Halite 0.02 mol/Lgw for all depths
        Calcite 0.0     0.75
        Gypsum  0.0     0.02
        Nahcolite       0.0     0.5
        Halite  0.0     0.02
SURFACE 1-20
# Site Density =  (1.92 umoles hydroxyl sites)/m^2 (assumed bidentate bonds)
#       from Davis and Kent (1990) and
#       used in Davis and Curtis (2003) Naturita GC Model
# Surface area (Mean of 10 values from 1-2 mm fraction) = 11.02 m^2/g (BET
Measurement)
# Used 7500 g rock/Lgw
# Of Total Sites: Very Strong Sites = 0.01 %, Strong Sites = 1.2 % (Davis and
Curtis)
# Total Sites = 158,688 umol sites/L gw  (from 7500*11.02*1.92)
# Very Strong Sites = 0.0001*158688 = 15.87 umoles/L (SJM Calculation)
# Strong Sites = 0.012 * 158688 = 1904 umoles/L  (SJM Calculation)
# Weak Sites = 0.9879 * 158688 = 156768 umoles/L  (SJM Calculation)
        -equilibrate 1
        Hfo_wOH         1.568e-1        11.02   7500.0
        Hfo_sOH         1.904e-3        11.02   7500.0
        Hfo_vOH         1.587e-5        11.02   7500.0
        -no_edl
PRINT
        -reset          true
ADVECTION
        -cells           20
        -shifts          200
        -punch           20
#        -punch           10 20
        -punch_frequency 1
        -print           20
        -print_frequency 50
USER_GRAPH
        -headings PV Na C NH4*5 Ca*10 Cl SO4 U*1000 KD*25000 pH*1000
#       -headings PV TOTADS CS TOT("U") KD
        -chart_title "Crescent Junction Vertical Transport Model"
        -axis_titles "PORE VOLUME" "Effluent Concentration (mg/L)"
        -axis_scale x_axis 0 10 1 0.1
        -axis_scale y_axis 0 25000.0 1000.0
        -initial_solutions false
        -plot_concentration_vs time
        -start
        5 TOTADS = MOL("Hfo_wOUO2OH") + MOL("Hfo_sOUO2CO3-") + MOL("Hfo_vOUO2OH") +
MOL("Hfo_vOUO2CO3-")
        6 CS = TOTADS/7500
        7 KD = (CS/TOT("U"))*1000
        10 GRAPH_X (STEP_NO + 0.5) / 20
        20 GRAPH_Y TOT("Na")*23000, TOT("C")*12000, TOT("Amm")*18000*5,
TOT("Ca")*40000*10, TOT("Cl")*35900, TOT("S(6)")*96000, TOT("U")*238000*1000,
KD*25000, 1000*(-LA"H+")
```

```
                                        Transport_vertical
#       20 GRAPH_Y TOT("U")*238000*1000, KD*25000
        -end
PRINT
        -user_graph true
SELECTED_OUTPUT
        -file              CJ_transport.sel
        -totals            Na Amm K Ca Cl
        -molalities                NaX AmmHX KX CaX2
END
```

Appendix H

Thermodynamic Database Used for PHREEQC Models

```
SOLUTION_MASTER_SPECIES
# PHREEQC Database modified with Jim Davis model used in Naturita GC Model
# See Davis and Curtis (2003)
# Removed all elements/species not used in models
#element        species alk     gfw_formula     element_gfw
#
H               H+      -1.0    H               1.008
H(0)            H2      0.0     H
H(1)            H+      -1.0    0.0
E               e-      0.0     0.0             0.0
O               H2O     0.0     O               16.0
O(0)            O2      0.0     O
O(-2)           H2O     0.0     0.0
Ca              Ca+2    0.0     Ca              40.08
Mg              Mg+2    0.0     Mg              24.312
Na              Na+     0.0     Na              22.9898
K               K+      0.0     K               39.102
Cl              Cl-     0.0     Cl              35.453
C               CO3-2   2.0     HCO3            12.0111
C(+4)           CO3-2   2.0     HCO3
Alkalinity      CO3-2   1.0     Ca0.5(CO3)0.5   50.05
S               SO4-2   0.0     SO4             32.064
S(6)            SO4-2   0.0     SO4
N               NO3-    0.0     N               14.0067
N(+5)           NO3-    0.0     N
Amm             AmmH+   0.0     AmmH            17.0
U               UO2+2   0.0     238.0290        238.0290
U(6)            UO2+2   0.0     238.0290        238.0290

SOLUTION_SPECIES

H+ = H+
        log_k   0.0
        -gamma  9.0     0.0

e- = e-
        log_k   0.0

H2O = H2O
        log_k   0.0

Ca+2 = Ca+2
        log_k   0.0
        -gamma  5.0     0.1650

Mg+2 = Mg+2
        log_k   0.0
        -gamma  5.5     0.20

Na+ = Na+
        log_k   0.0
        -gamma  4.0     0.075

K+ = K+
        log_k   0.0
        -gamma  3.5     0.015

Cl- = Cl-
        log_k   0.0
        -gamma  3.5     0.015

CO3-2 = CO3-2
        log_k   0.0
```

```
        -gamma  5.4     0.0

SO4-2 = SO4-2
        log_k   0.0
        -gamma  5.0     -0.04

NO3- = NO3-
        log_k   0.0
        -gamma  3.0     0.0

AmmH+ = AmmH+
        log_k   0.0
        -gamma  2.5     0.0

#UO2+2 primary master species
        UO2+2 = UO2+2
        log_k           0.0

H2O = OH- + H+
        log_k   -14.0
        delta_h 13.362  kcal
        -analytic       -283.971        -0.05069842     13323.0 102.24447
-1119669.0
        -gamma  3.5     0.0

#O2 secondary master species
        2H2O = O2 + 4H+ + 4e-
        log_k           -86.08
        delta_h 134.79 kcal

#H2 secondary master species
        2 H+ + 2 e- = H2
        log_k           -3.15
        delta_h -1.759

########################################################################
#MAJOR ION SPECIES FROM DAVIS AND CURTIS NRC REPORT TABLE 2-1. 2003
CO3-2 + H+ = HCO3-
        log_k   10.329

CO3-2 + 2 H+ = CO2 + H2O
        log_k   16.683

SO4-2 + H+ = HSO4-
        log_k   1.98


########################################################################


AmmH+ = Amm + H+
        log_k   -9.252
        delta_h 12.48   kcal

AmmH+ + SO4-2 = AmmHSO4-
        log_k   1.11

Ca+2 + H2O = CaOH+ + H+
        log_k   -12.78

Ca+2 + CO3-2 = CaCO3
        log_k   3.224
```

```
Ca+2 + CO3-2 + H+ = CaHCO3+
        log_k   11.435

Ca+2 + SO4-2 = CaSO4
        log_k   2.3

Mg+2 + H2O = MgOH+ + H+
        log_k   -11.44

Mg+2 + CO3-2 = MgCO3
        log_k   2.98

Mg+2 + H+ + CO3-2 = MgHCO3+
        log_k   11.399

Mg+2 + SO4-2 = MgSO4
        log_k   2.37

Na+ + H2O = NaOH + H+
        log_k   -14.18

Na+ + CO3-2 = NaCO3-
        log_k   1.27

Na+ + HCO3- = NaHCO3
        log_k   -0.25

Na+ + SO4-2 = NaSO4-
        log_k   0.7

K+ + H2O = KOH + H+
        log_k   -14.46

K+ + SO4-2 = KSO4-
        log_k   0.85

#URANIUM SPECIES FROM TABLE 2-1 DAVIS AND CURTIS NRC REPORT 2003

#UO2OH+
        UO2+2 + H2O = UO2OH+ + H+
        log_k           -5.20

#UO2(OH)2
        UO2+2 + 2 H2O = UO2(OH)2 + 2H+
        log_k           -11.5

#UO2(OH)3-
        UO2+2 + 3H2O = UO2(OH)3- + 3H+
        log_k           -20.00

#UO2(OH)4-2
        UO2+2 + 4H2O = UO2(OH)4-2 + 4H+
        log_k           -33.0

#(UO2)2OH+3
        2UO2+2 + H2O = (UO2)2OH+3 + H+
        log_k           -2.70

#(UO2)2(OH)2+2       597
        2UO2+2 + 2H2O = (UO2)2(OH)2+2 + 2H+
        log_k           -5.62

#(UO2)3(OH)4+2
```

```
        3UO2+2 + 4H2O = (UO2)3(OH)4+2 + 4H+
        log_k           -11.90

#(UO2)3(OH)5+          598
        3UO2+2 + 5H2O = (UO2)3(OH)5+ + 5H+
        log_k           -15.55

#(UO2)3(OH)7-
        3UO2+2 + 7H2O = (UO2)3(OH)7- + 7H+
        log_k           -31.00

#(UO2)4(OH)7+
        4UO2+2 + 7H2O = (UO2)4(OH)7+ + 7H+
        log_k           -21.90

#UO2CO3                603
        UO2+2 + CO3-2 = UO2CO3
        log_k           9.67

#UO2(CO3)2-2           604
        UO2+2 + 2CO3-2 = UO2(CO3)2-2
        log_k           16.94

#UO2(CO3)3-4           605
        UO2+2 + 3CO3-2 = UO2(CO3)3-4
        log_k           21.60

#(UO2)3(CO3)6-6        648
        3UO2+2 + 6CO3-2 = (UO2)3(CO3)6-6
        log_k           54.0

#(UO2)2CO3(OH)3-
        2UO2+2 + CO3-2 + 3H2O = (UO2)2CO3(OH)3- + 3H+
        log_k           -0.86

#(UO2)3CO3(OH)3+
        3UO2+2 + CO3-2 + 3H2O = (UO2)3CO3(OH)3+ + 3H+
        log_k           0.66

#(UO2)11(CO3)6(OH)12-2
        11UO2+2 + 6CO3-2 + 12H2O = (UO2)11(CO3)6(OH)12-2 + 12H+
        log_k           36.43

#UO2NO3+               646
        UO2+2 + NO3- = UO2NO3+
        log_k           0.3

#UO2Cl+                611
        UO2+2 + Cl- = UO2Cl+
        log_k           0.17
#       delta_h 1.9 kcal

#UO2Cl2                644
        UO2+2 + 2Cl- = UO2Cl2
        log_k           -1.1
#       delta_h 3.6 kcal

#UO2SO4                612
        UO2+2 + SO4-2 = UO2SO4
        log_k           3.15
        delta_h 4.7 kcal

#UO2(SO4)2-2           613
```

```
        UO2+2 + 2SO4-2 = UO2(SO4)2-2
        log_k           4.14
        delta_h 8.4 kcal


PHASES

Calcite
        CaCO3 = CO3-2 + Ca+2
        log_k   -8.48
        delta_h -2.297 kcal
        -analytic       -171.9065       -0.077993       2839.319        71.595

Aragonite
        CaCO3 = CO3-2 + Ca+2
        log_k   -8.336
        delta_h -2.589 kcal
        -analytic       -171.9773       -0.077993       2903.293        71.595

Dolomite
        CaMg(CO3)2 = Ca+2 + Mg+2 + 2 CO3-2
        log_k   -17.09
        delta_h  -9.436 kcal

Gypsum
        CaSO4:2H2O = Ca+2 + SO4-2 + 2 H2O
        log_k   -4.58
        delta_h -0.109 kcal
        -analytic       68.2401 0.0     -3221.51        -25.0627

Anhydrite
        CaSO4 = Ca+2 + SO4-2
        log_k   -4.36
        delta_h -1.710 kcal
        -analytic       197.52  0.0     -8669.8 -69.835

Halite              64
        NaCl = Na+ + Cl-
        log_k           1.582
        delta_h 0.918 kcal

Thenardite          65
        Na2SO4 = 2Na+ + SO4-2
        log_k           -0.179
        delta_h -0.572 kcal

Nahcolite           58
        NaHCO3 = Na+ + HCO3-
        log_k           -0.548
        delta_h 3.720 kcal

Trona               59
        NaHCO3:Na2CO3:2H2O = 2H2O + 3Na+ + CO3-2 + HCO3-
        log_k           -0.795
        delta_h -18.0 kcal

Natron              60
        Na2CO3:10H2O = 2Na+ + CO3-2 + 10H2O
        log_k           -1.311
        delta_h 15.745 kcal

Thermonatrite       61
        Na2CO3:H2O = 2Na+ + CO3-2 + H2O
```

```
        log_k           0.125
        delta_h -2.802 kcal
#############################################################
# Uranium Mineral FROM TABLE 2-2 DAVIS AND CURTIS NRC REPORT 2003

Schoepite           602
        UO2(OH)2:H2O + 2H+ = UO2+2 + 3H2O
        log_k           4.93

Rutherfordine       606
        UO2CO3 = UO2+2 + CO3-2
        log_k           -14.49

Gummite             600
        UO3 + 2H+ = UO2+2 + H2O
        log_k           10.403
        delta_h -23.015 kcal

UO3(gamma)              599
        UO3 + 2H+ = UO2+2 + H2O
        log_k           7.719
        delta_h -19.315 kcal

#############################################################################################


Na4UO2(CO3)3        571
        Na4UO2(CO3)3 = 4Na+ + UO2+2 + 3CO3-2
        log_k           -16.290

B-UO2(OH)2          601
        UO2(OH)2 + 2H+ = UO2+2 + 2H2O
        log_k           5.544
        delta_h -13.730 kcal


#############################################################
# CO2 gas FROM TABLE 2-1 DAVIS AND CURTIS NRC REPORT 2003

CO2(g)
        CO2 = CO2
        log_k   -1.472
#       delta_h -4.776 kcal
#       -analytic       108.3865        0.01985076      -6919.53        -40.45154
669365.0
#############################################################

H2O(g)
        H2O = H2O
        log_k           1.51
        delta_h         -44.03   kJ
#    Stumm and Morgan, from NBS and Robie, Hemmingway, and Fischer (1978)

# Gases from LLNL.dat...


Amm(g)
        Amm = Amm
        log_k           1.7966


EXCHANGE_MASTER_SPECIES
        X       X-
```

```
EXCHANGE_SPECIES
        X- = X-
        log_k   0.0

        Na+ + X- = NaX
        log_k   0.0
        -gamma  4.0     0.075

        K+ + X- = KX
        log_k   0.7
        -gamma  3.5     0.015
        delta_h  -4.3   # Jardine & Sparks, 1984

# !!!!!
#       H+ + X- = HX
        log_k   1.0
        -gamma  9.0     0.0

        AmmH+ + X- = AmmHX
        log_k   0.6
        -gamma  2.5     0.0
        delta_h  -2.4   # Laudelout et al., 1968

        Ca+2 + 2X- = CaX2
        log_k   0.8
        -gamma  5.0     0.165
        delta_h  7.2    # Van Bladel & Gheyl, 1980

        Mg+2 + 2X- = MgX2
        log_k   0.6
        -gamma  5.5     0.2
        delta_h  7.4    # Laudelout et al., 1968

############################################################
# Surface Species FROM TABLE 5.4 DAVIS AND CURTIS NRC REPORT 2003
SURFACE_MASTER_SPECIES
        Hfo_v   Hfo_vOH
        Hfo_s   Hfo_sOH
        Hfo_w   Hfo_wOH
############################################################
SURFACE_SPECIES

# Very strong binding site Hfo_ss
# Strong binding site  Hfo_s
# Weak binding site  Hfo_w

        Hfo_vOH = Hfo_vOH
        log_k   0.0

        Hfo_sOH = Hfo_sOH
        log_k   0.0

        Hfo_wOH = Hfo_wOH
        log_k   0.0

############################################################
# Uranium Surface Species FROM TABLE 5.4 DAVIS AND CURTIS NRC REPORT 2003
# Uranyl
        Hfo_wOH + UO2+2 + H2O = Hfo_wOUO2OH + 2H+
        log_k  -6.74

        Hfo_sOH + UO2+2 + CO2 + H2O = Hfo_sOUO2CO3- + 3H+
        log_k  -8.00
```

```
        Hfo_vOH + UO2+2 + H2O = Hfo_vOUO2OH + 2H+
        log_k   -2.06

        Hfo_vOH + UO2+2 + CO2 + H2O = Hfo_vOUO2CO3- + 3H+
        log_k   -6.36
#############################################################

END
```