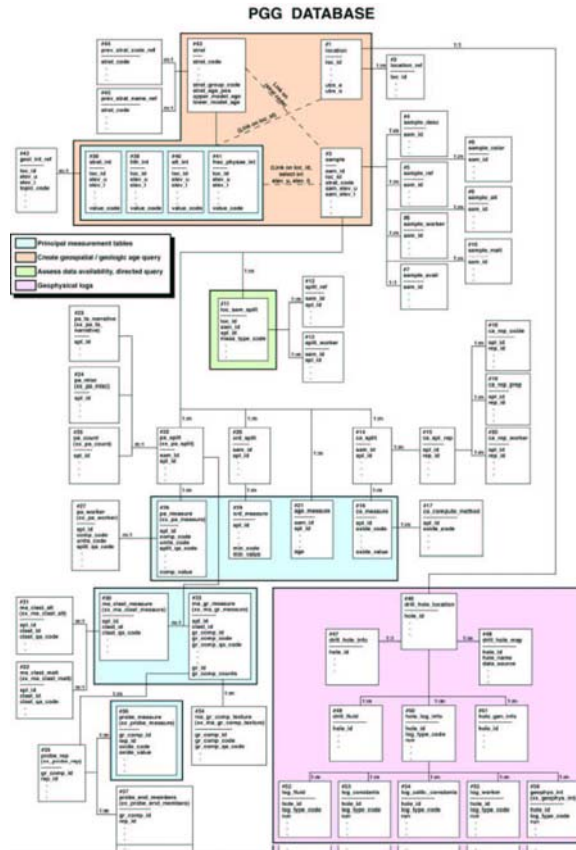# A PETROGRAPHIC, GEOCHEMICAL, AND GEOPHYSICAL DATABASE, AND STRATIGRAPHIC FRAMEWORK FOR THE SOUTHWESTERN NEVADA VOLCANIC FIELD

Richard G. Warren, David A. Sawyer, Frank M. Byers, Jr. and Gregory L. Cole
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contributors Scott A. Minor, Mark R. Hudson, James C. Cole, David E. Broxton, Keith Roberson, Tom E. Garrison, Emily C. Kluk, George H. Juniel II, Brian M. Allen, Sigmund L. Drellack, Jr., Susan H. Freeman, David T. Vaniman, David A. Mann, Jeffrey L. Wagoner, and Robert J. Fleck

Los Alamos
NATIONAL LABORATORY

A PETROGRAPHIC, GEOCHEMICAL, AND GEOPHYSICAL DATABASE, AND
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Abstract

The legacy of the Cold War includes voluminous geological information collected to support activities related to the underground testing of nuclear devices. The Nevada Test Site was the primary location for U.S. testing and coincides with the eastern half of the 10,000 km^2 southwestern Nevada volcanic field. The geology of this volcanic field has been intensely characterized for a period exceeding 30 years, initially to support nuclear containment activities, and more recently to support environmental restoration and nuclear waste disposal. Available information includes surface and subsurface geology, stratigraphy and age dating, geochemistry, petrography, mineralogy, and physical and geophysical measurements. While the collected data continue to have an important role for Test Site activities, they have a much broader application within the geoscience community.

We have integrated geological information generated to support nuclear testing into a large, relational database. These data were generated primarily by Los Alamos National Laboratory and by the U.S. Geological Survey, and partly obtained from published literature. The database is particularly robust in petrographic analyses, and introduces new techniques devised to provide precise and accurate analyses for minor and trace constituents, with detailed documentation. This petrographic work allows definition of the intimate relation of optical mineralogy to chemistry and mineral identification via electron microprobe analysis. The database also defines the subsurface geology of the test site areas through "geologic interval" data tables, which provide stratigraphic assignments, lithologies, alterations, and other characteristics for more than 750 drill holes within the region. Geophysical logs from approximately 400 drill holes have been added to the database in its first revision.

This digital database is served by the Geographic Information System (GIS) Team at Los Alamos National Laboratory, and can be accessed there through the Internet on the website of Earth and Environmental Sciences (EES). Selected information can be extracted from the database with spatial (X, Y, Z) and temporal (age or stratigraphy) attributes, to evaluate schemes for predictive analysis and modeling at the Nevada Test Site, with possible application to other geologic environments.

This document is meant to be a companion to the database, which can be downloaded or accessed through the Internet. We hope that the great volume of complex, interrelated data and data types within this data set will encourage non-petrographers, non-geologists, or others to utilize these data for testing and development of geological or hydrogeologic models, statistical methods, data mining techniques, exploratory data analysis, and visualization techniques.

I. INTRODUCTION AND HISTORY OF THE DATABASE

The Nevada Test Site is situated within a 10,000-km2 province called the southwestern Nevada volcanic field (SWNVF) by Christiansen et al. (1977). The SWNVF contains multiple suites of Miocene silicic volcanic rocks, erupted from an evolving system of calderas (Figure 1). The volcanic rocks overlie a basement of Paleozoic sedimentary rocks. The general geologic framework and history of important work for this volcanic field are summarized by Byers et al. (1989). Collection of detailed geological information to support activities of the Nevada Test Site (NTS) began in the 1960's. Geoscientists from Los Alamos National Laboratory (LANL), Lawrence Livermore National Laboratory (LLNL), the U.S. Geological Survey (USGS), and various government contractors, particularly Raytheon Services Nevada (RSN), conducted numerous studies of the geologic framework to assist in the safe underground testing of nuclear devices. Development and appropriate integration of the geologic framework into testing activities resulted in successful geological containment of radionuclides from the underground tests. The surface expression of the underground testing can be seen in the photograph of Figure 2.
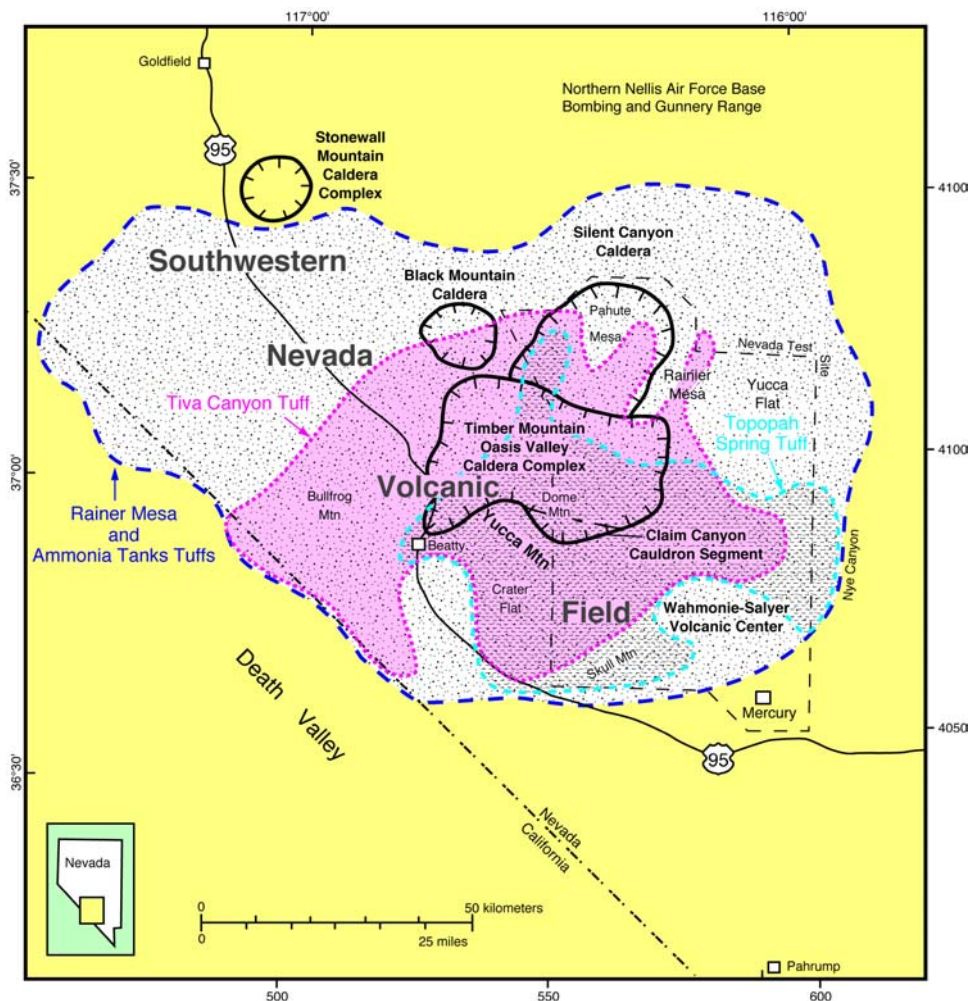
Figure 1. Calderas within the SWNVF (from Warren et al., 1989b), showing areal extents of large-volume ash-flow sheets. This representation is taken mostly from Byers et al. (1976b), with the addition of the Stonewall Mountain caldera complex described by Noble et al. (1984). More recent work by Carr et al. (1986), Noble et al. (1991), and Ferguson et al. (1994) have expanded, somewhat modified, or presented alternatives to this view. Values shown on the right and bottom margins of the figure represent UTM coordinates in kilometers.
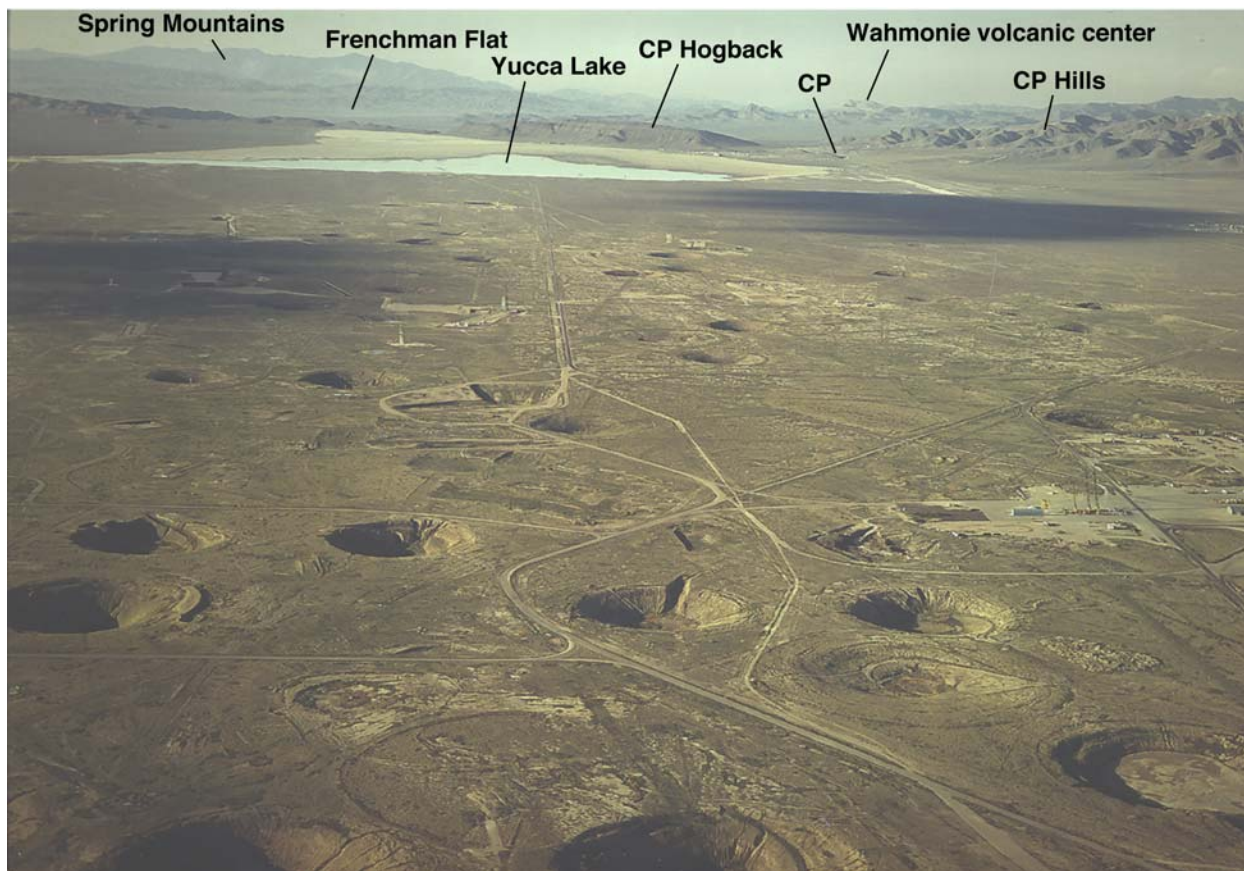
Figure 2. Collapse features within Yucca Flat testing area of the Nevada Test Site, viewing to south. The vaporization of an enormous volume of rock during an underground nuclear explosion creates a void into which overlying rocks generally collapse. Ironically, collapses that reach the surface seal off any geologically available pathway for the release of radionuclides, and effectively guarantee underground containment of all radioactive gases produced by the nuclear explosion.

Geological data provided in this database were generated primarily by personnel of LANL and the USGS. Other organizations also retain datasets containing geological information obtained from samples collected within the SWNVF, both in hard copy and in electronic form.

Los Alamos National Laboratory has played a major role in testing activities. Geoscientists at LANL assembled various types of geological and geophysical data to support containment science for the safe underground testing of nuclear devices. Details of the evolution of geologic data and model development in support of the Containment program are provided in Appendix A. The geological data provided within the database were originally assembled beginning in 1987 within a non-relational database. General usage of these geological data in this form was difficult because of the reliance on proprietary software and operating systems, and the non-relational format of much of the data. Standardization of operating systems (to UNIX and WINDOWS), development of the Structured Query Language (SQL) standard for relational databases, and the availability of commercial SQL-compliant database implementations provided a strong incentive for the authors to restructure and reformat the geological data for input into an SQL-compliant database. The geophysical data formerly constituted the primary basis of the GEODES database (Winterkamp et al., 1985). With the addition of the geophysical data from GEODES to the original database (Warren et al., 2000), all these data now reside in a set of relational tables served by the Geographic Information System Laboratory (GISLab) facility in the Earth and Environmental Sciences

Division at LANL. This revised database is maintained for public access through the internet at a site maintained by GISLab.

II. THE GEOLOGICAL DATA

The geological data are organized within a set of related database tables. These tables are described in this section; beginning with tables defining attributes for the measurement location, followed by those containing the geological measurements. Database table names are identified by italics within the text. For example, *table_desc* is a table that contains descriptions of individual tables and their data fields. The relational structure and organization of these tables are described in the next section.

Tables within each of the following subsections identify the database tables that support the identified data items. These tables describe the contents and associated tables (foreign keys) for each of the named database tables. The term foreign key has its origin in relational database literature and is a table that provides a list of acceptable values for a given data field within a database table.

Locations and Samples

Geologic measurements and supporting information are provided for depth (elevation) intervals of more than 750 drill holes, and for points at approximately 4,300 surface and subsurface locations within the database tables listed in Table 1. Geological interval measurements are descriptive (text data), whereas geophysical interval measurements are quantitative (numeric data). Separate tables for the different data types identify the type of laboratory measurement as well as its value. More than 8,600 samples (point data) were collected at the 4,300 locations, and multiple splits (e.g. X-ray diffraction, polished thin section, wet chemistry) often provide a diversity of measurements for individual samples. Most of the "point" measurement data are reported at the split-level, with the associated table structures reflecting the generic class of laboratory data (e.g. chemical, petrologic, mineralogic). The quantitative measurements are provided with the appropriate units of measure and individual uncertainty values, if available. Most samples used for these splits have been curated and are available for additional work. The different types of laboratory measurements are described in the following sections.

Primary laboratory measurements reported at the split-level are contained in database tables with names that begin with a code reflecting the generic class of data, and end in *_measure*, e.g., *ca_measure*, which contains data for chemical analyses and *pa_measure*, which contains data for petrographic analyses. Multivalued descriptive information that constitutes primary measurements is most efficiently stored in separate tables, such as *sample_alt* (Table 1). Multivalued, descriptive information for each measurement is stored within separate database tables whose names begin with the same generic class code, e.g., *sample_worker*. Such supporting information is often termed metadata . These different types of tables are described in the *geological database* section.

Table name	Description	Foreign key tables
location	Describes sample locations	loc_qa_ list, quad_ list
location_ref	Sources of information for location	topic_list, ref_list
sample	Sample characteristics	strat_list, sam_type_list, lit_list
sample_desc	Sample descriptions	worker_list, sam_desc_type_list
sample_ref	Citations for sample characteristics	topic_list, ref_list
sample_worker	Sample workers	topic_list, worker_list
sample_avail	Sample availability	avail_list
sample_color	Sample colors	comp_list, hue_list
sample_alt	Alteration of sample	alt_list
sample_malt	Minor alteration of sample	alt_list

Table 1. Database tables for locations and samples. More detailed descriptions of each table are provided in database table *table_desc*.

Age Dates and Stratigraphic Units

Age measurements, determined primarily by the Ar/Ar and K/Ar dating methods, are available for 386 samples within database tables listed in Table 2. These measurements provide model ages for Tertiary units of the SWNVF, which constitute the vast majority of the 365 stratigraphic units or subunits defined within the SWNVF. Figure 3 shows a portion of the stratigraphic column that is based on these age assignments. The assigned stratigraphic codes define groups of petrographically, chemically, and temporally related units (Warren et al., 1989a). These groups are termed "volcanic assemblages".

Table name	Description	Foreign key tables
age_measure	Age date	split_type_list, comp_list
Strat	Stratigraphic units	strat_list
prev_strat_code_ref	References for previously used stratigraphic symbols	strat_list, ref_list
prev_strat_name_ref	Reference codes for previously used stratigraphic names	strat_list, ref_list

Table 2. Database tables for age dates and stratigraphic units.
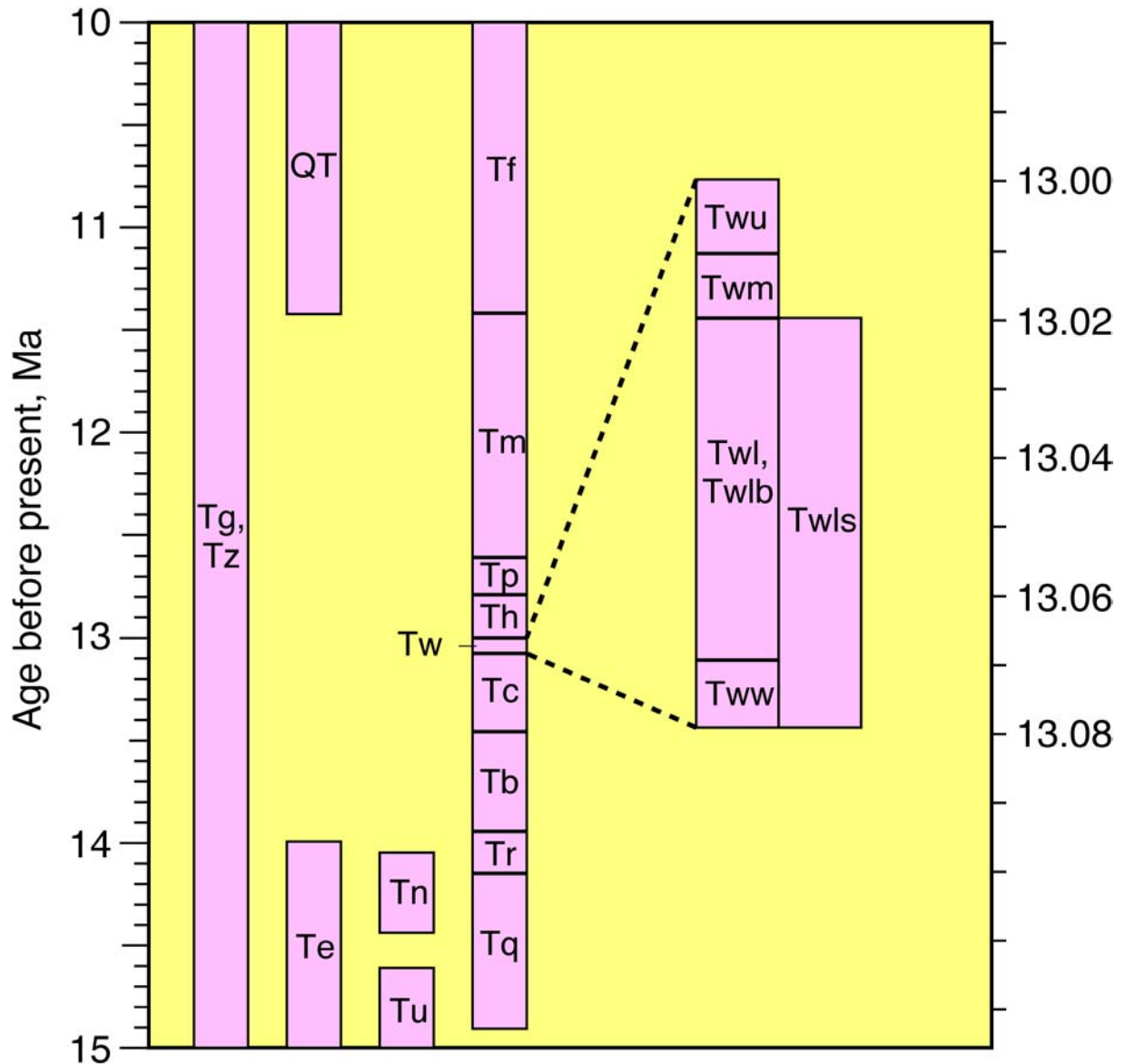
Figure 3. Stratigraphic column for assemblages of the SWNVF emplaced between 10 to 15 Ma. Voluminous caldera-related silicic volcanism occurred between 16.3 to 11.4 Ma from the centers shown in Figure 1 and from additional centers of unknown location buried by younger volcanism. Stratigraphic codes used in the column (e.g. QT, Tf) identify stratigraphic units as defined in database table *strat*. Individual units are shown for the Wahmonie Formation (Tw), using the expanded scale of model ages shown to the right.

Chemical Analyses

Chemical analyses are provided for nearly 3,000 samples within the database tables listed in Table 3. More than 80,000 chemical concentrations, representing 70 of the 85 natural occurring elements, have been obtained by a variety of analytical methods such as X-ray fluorescence (XRF), neutron activation analysis (NAA), and a variety of wet chemical methods such as atomic absorption, flame emission spectroscopy, and inductively-coupled plasma emission spectroscopy. Each sample split normally reflects a general analytical type, although sample preparation, computational method, and analytical

"subtype" can vary for individual analytes. For example, a wet chemical split could include analyses by the subtypes atomic absorption, flame or inductively-coupled plasma emission spectroscopy, or gravimetric analysis. Multiple splits from a sample can provide multiple measurements for a single analyte. Database tables described in Table 3 provide supplemental information so that users can make informed decisions regarding which data are most appropriate for their use. For all elements, concentrations are reported as the oxide that generally predominates in the natural environment, for example, MgO and BaO. Note that a trace element such as Ba is typically reported as the element rather than the oxide within the geochemical literature. Concentrations can be converted to elemental form through use of a foreign key table of gravimetric factors. Many chemical data represent the average of repeat analyses (replicates) of a split by the same technique, occasionally performed on a different day and/or by another analyst. Because of this, sample preparation and analyst data are stored in separate replicate tables to allow the many-to-one relationship between such replicate data and the reported chemical measurements to be preserved.

Table name	Description	Foreign key tables
ca_split	Chemical analysis type	split_type_list, meas_type_list
ca_spl_rep	Replicate ID	
ca_measure	Chemical data	oxide_list, error_meth_list, units_list, ca_subtype_list, ref_list
ca_compute_method	Computational method	ca_comp_meth_code
ca_rep_oxide	Replicate analyte	oxide_list
ca_rep_prep	Sample preparation	ca_prep_list
ca_rep_worker	Chemical analyst	worker_list

Table 3. Database tables for chemical analyses (ca).

Many of the previously unpublished chemical analyses in the database were generated within the Earth and Environmental Sciences (EES) XRF laboratory at LANL (Figure 4). All splits are prepared as fused disks by fusing the sample with a low-Z (lithium borate) flux, which dilutes the sample, minimizing matrix affects. The model used to calculate concentrations from measured X-ray intensities is non-linear, utilizes loss on ignition (LOI), and is based on more than 40 standards, with reference analytical values mostly from Govindaraju (1994). Use of LOI in computations is important because loss of volatiles during fusion changes the initially measured flux to sample ratio. This computational model provides realistic estimates of uncertainty in the accuracy of these XRF analyses.

Figure 4. The XRF instrument at LANL. A) Panel for display of elements currently being analyzed and their count rates, B) Operation control panel, C) Control panel for sample changer, D) Automatic sample changer, E) Chart recorder for wavelength scans of X-ray intensities.

Petrographic Analyses

Nearly 90,000 quantitative mineral abundances have been obtained by optical petrography for nearly 4700 samples. These analyses are compiled within database tables listed in Table 4. Supplemental descriptive information provided for each analysis includes mineral alteration. Analyses of individual minerals, described in the next section, supplement and support many petrographic analyses. Measurements are available from four general types of petrographic methods, several representing new petrographic methods. The methods, described below, include grain mount analyses, "quick look" estimates, "standard" analyses by point count, and "detailed" analyses. Some samples have been analyzed by more than one method.

Table name	Description	Foreign key tables
pa_split	General petrographic information	split_type_list, pa_meth_list, light_type_list, comp_list, sep_meth_list, qa_list
pa_misc	Miscellaneous petrographic information	pa_meas_type_list, qa_list
pa_count	Points counted for petrographic analysis	pa_meth_list, qa_list
pa_measure	Petrographic analyses	comp_list, units_list, comp_alt_list, pa_meth_list, ref_list, qa_list
pa_worker	Petrographic analyst	comp_list, worker_list, qa_list
xx_pa_split	Superceded or erroneous general petrographic information	split_type_list, pa_meth_list, light_type_list, comp_list, sep_meth_list, qa_list
xx_pa_misc	Superceded or erroneous miscellaneous petrographic information	pa_meas_type_list, qa_list
xx_pa_count	Superceded or erroneous points counted for petrographic analysis	pa_meth_list, qa_list
xx_pa_measure	Superceded or erroneous petrographic analyses	comp_list, units_list, comp_alt_list, pa_meth_list, ref_list, qa_list
xx_pa_worker	petrographic analyst for superceded or erroneous analysis	comp_list, worker_list, qa_list

Table 4. Database tables for petrographic analyses (pa). Tables with names that begin *xx_* should not be employed for usual applications of petrographic data.

Our technique for grain mount analysis provides an accurate measure for the relative proportions of felsic phenocrysts (quartz and feldspars), crude measures for abundances of other constituents, and a microscopic view of sample alteration. The method provides inexpensive, quantitative petrographic information and avoids delays associated with thin section preparation. With a petrographic microscope stationed at a drill rig, petrographic data can be immediately available for critical drilling decisions. The method generates quantitative data comparable in accuracy to analysis of a thin section (Table 5). Our technique provides quantitative analysis only for felsic minerals and does not provide a permanent sample, as does standard thin section analysis. The grain mount analysis proceeds by crushing a few grams of sample in a mortar to silt size, pinching a few milligrams of this powder between the thumb and forefinger, and sprinkling the powder on a standard thin section slide. After adding a drop or two of immersion oil and covering the oil with a cover slip, the sample is ready for grain mount analysis.

"Quick look" estimates provide crude but useful petrographic data when time or expense is a primary consideration. The accuracy of individual quick look estimates reflect the effort for each such analysis, which varies widely. Each quick look analysis ranges from a five minute inspection of the thin section to estimation of abundances from detailed photodocumentation of the largest mineral grains, as described below. Comparing superceded quick look analyses with detailed analyses of the same thin section demonstrates that the quick look estimates are generally only slightly less accurate for the relative proportion of felsic phenocrysts. Quick look estimates are generally accurate within a factor of two for the total abundance of felsic phenocrysts, and within a factor of three for abundances of mafic phenocrysts (biotite, hornblende, pyroxene, olivine). Although these uncertainties are indeed large, the differences in mineral abundances among stratigraphic units are often several times larger. These data can therefore be very useful for certain applications.

Most of the "standard" petrographic analyses of this database are based on very accurate and precise identification (counts) of minerals using a very large number of grid points for each thin section, and so may be standard in their methodology but with much higher accuracy and precision than normally reported for this type of analysis. Points were generally counted at 0.1 mm intervals within traverse lines separated by 0.5 or 1.0 mm, covering as much of the thin section as a standard point counting stage would allow, generally 90-100% of the slide. With this approach, precision is adequate for minor constituents, including mafic minerals and Fe-Ti oxide minerals (magnetite and ilmenite).

Felsic phenocryst	Petrographic method	Mafic-poor Calico Hills Formation (Thp)				Rhyolite of Echo Peak (Tpe)		
		value	2SEM	n		value	2SEM	n
Total felsic phenocrysts (volume %)	*Point count*	2.3	0.2	176		8.9	1.1	27
	Grain mount	2.4	0.4	71		6.5	1.3	4
	Quick look	3.4	0.4	71		12.6	1.1	30
Quartz (percent of felsic phenocrysts)	*Point count*	41	2	148		0.4	0.4	27
	Grain mount	42	4	54		2.7	1.6	19
	Quick look	40	2	67		0.9	0.5	30
K-spar (percent of felsic phenocrysts)	*Point count*	35	2	148		65	4	27
	Grain mount	41	3	54		64	4	19
	Quick look	41	3	67		58	3	30
Plagioclase (percent of felsic phenocrysts)	*Point count*	25	2	148		35	4	27
	Grain mount	17	2	54		33	4	19
	Quick look	20	3	67		41	3	30

Table 5. Comparison of mean values obtained by different petrographic methods. Statistical parameters are twice the standard error of the mean (2SEM) and number of analyses (n). Includes only analyses entered into database by 23 October 1998. Values from *point count* are the most accurate. Values from *grain mount* provide analyses that compare well with those from *point count*. A typically slightly higher content of quartz from *grain mount* analysis is attributed to a contribution of quartz from phenocrysts and coarse granophyric groundmass within lithics. Values for total felsic phenocrysts from *quick look* are typically erroneously high compared to those from *point count*. Stratigraphic units compared are mafic-poor Calico Hills Formation (Thp) and rhyolite of Echo Peak (Tpe), which occur in succession within certain areas of Pahute Mesa subsurface. Some non-representative samples from these units are not included in the comparison.

All "detailed" petrographic analyses in this database were performed by Rick Warren, using methods he developed to provide thoroughly documented petrographic analyses for minor and accessory minerals. These methods require that individual components be located on a "photomap" of a polished thin section, and their mineral identities, textures, and other features noted on standardized worksheets (Figure 5). Application of this technique requires combined use of reflected and transmitted light, with grain margins determined in reflected light to assure point counting on a truly planar surface without depth of field.
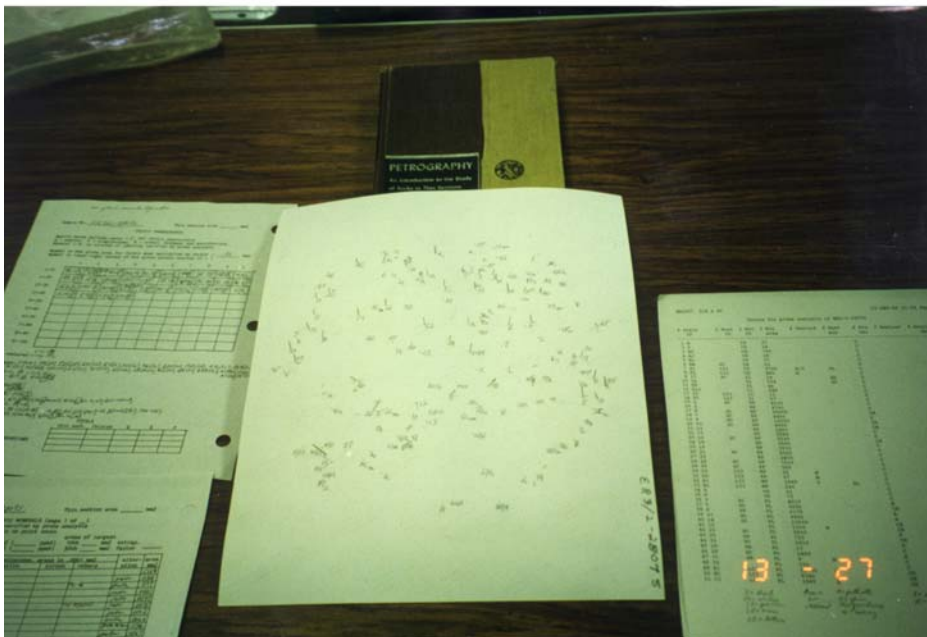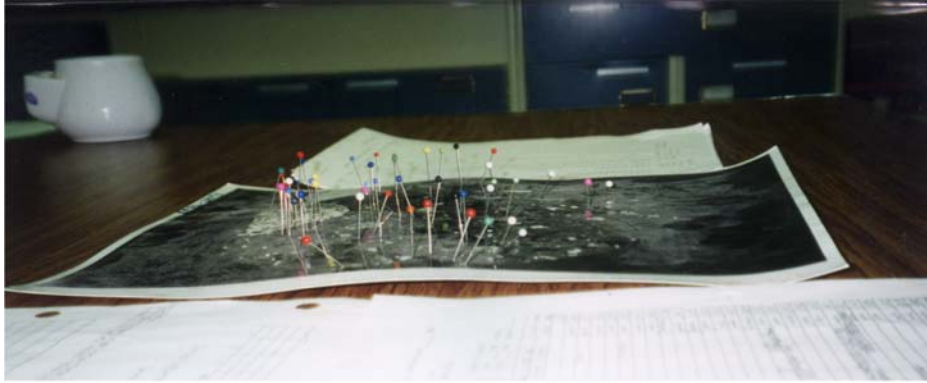
Figure 5. Photomaps and petrographic worksheets used for detailed petrographic analysis.

All detailed analyses require systematic scans of the entire polished thin section at 100X, first in reflected light, and then in transmitted light. Each scan consists of successive traverses across the entire length of the thin section, spaced 1.5 to 2.0 mm apart, with the field of view for each traverse, 1.7 to 2.2 mm, slightly overlapping that of the previous traverse. Traverses in transmitted light are offset from those in reflected light by 0.5 mm. Minerals intersected by the point count, those located during scans for the determination of their abundances, and components included to represent features of interest are marked with pins as shown in Figure 5. A point count usually precedes the systematic scans, but is not required for detailed analysis and is often omitted for crystal-poor samples. The pins are systematically removed from the photomap as the worksheet is completed. The worksheet is reduced into electronic form, and mineral abundances, based on the analytical method and mineralogic data from the worksheet, are determined through computer processing.

Except for sphene and allanite, which typically occur in larger grains, accessory grains either have a smaller thickness than the polished thin section or are wholly or partly included within opaque phases, making them virtually invisible in transmitted light (Figure 6). Consequently, abundances of most

accessory minerals are highly underestimated without use of reflected light. All accessory and minor minerals have distinctive reflectivities, assuring that all individual grains in a polished section can be recognized, as required by Method A (described below).
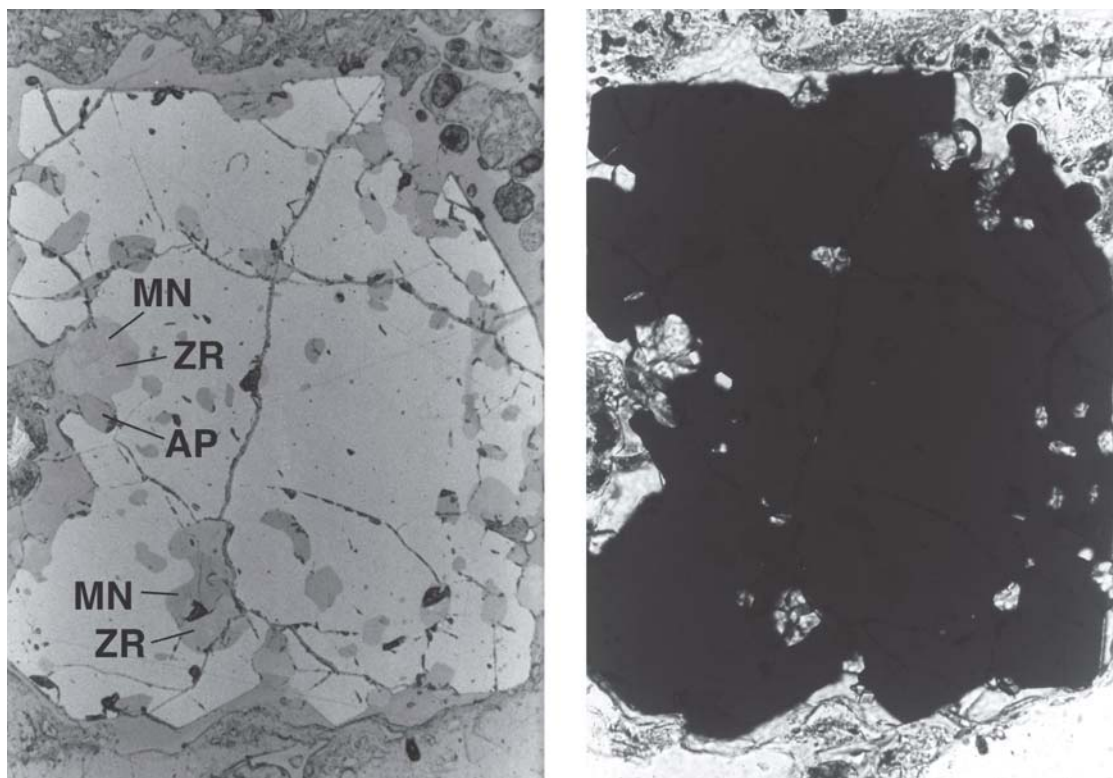
Figure 6. Reflected light (left) and transmitted light (right) views of ilmenite grain O4 in split RW19AK2 B. Field of view is approximately 0.5 mm by 0.7 mm. Most inclusions, with examples identified as zircon (ZR), apatite (AP), and monazite (MN), are invisible in transmitted light.

The methods of detailed petrographic analysis are described in detail within database table *pa_meth_list*. Methods *A, C,* and E are those most frequently employed for detailed petrographic analysis. Method A is the most commonly used to determine abundances of primary minerals that occur at <100 parts per million by volume (ppmV). Method C, a variation of Method A, is more practical to apply at higher abundances of apatite, zircon, or perrierite/chevkinite, and utilizes the observed linear relationship between the areal density of these three accessory minerals and their abundances, as illustrated in Figure 7. Method E is the most commonly applied detailed petrographic method to determine abundances of mafic minerals, particularly when their abundances are between 1000 to 10,000 ppmV (0.1 to 1%).
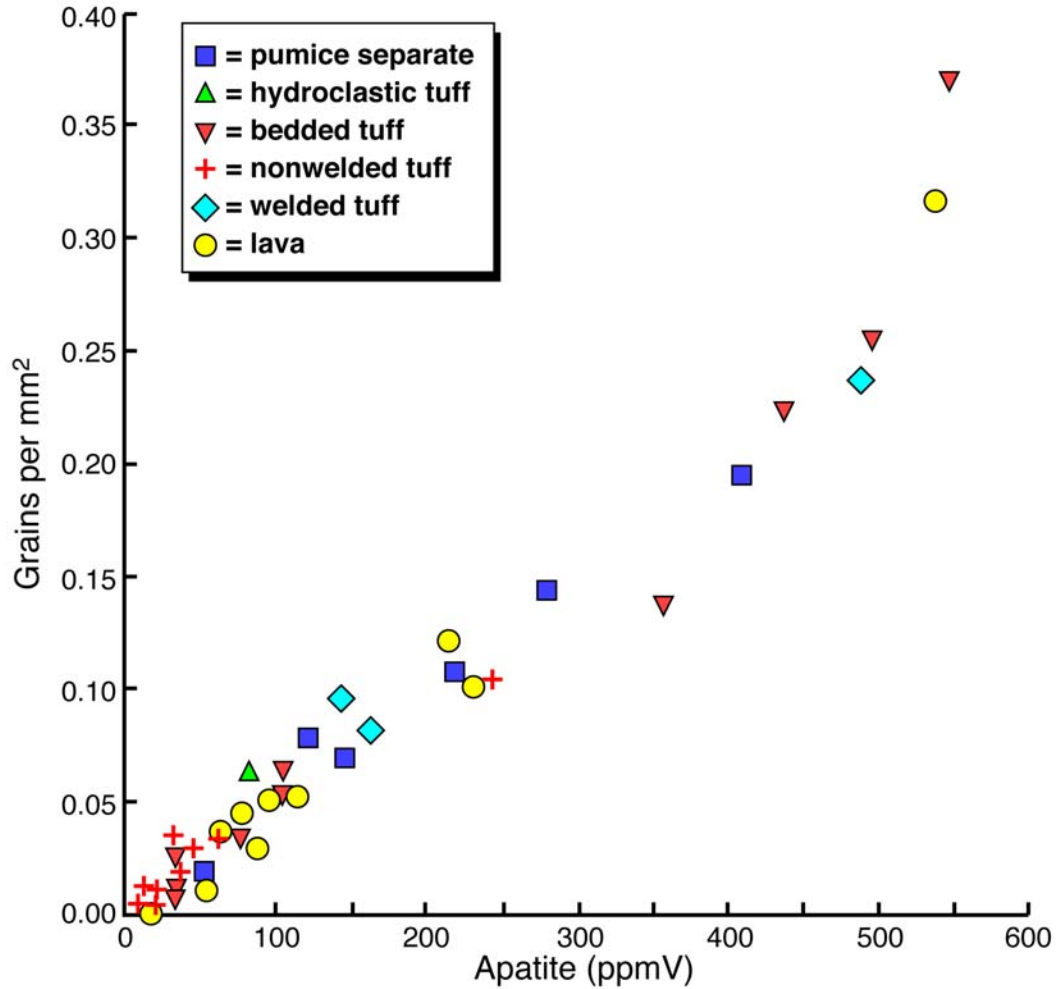
Figure 7. Apatite abundances determined by method *A* plotted versus the areal density of apatite grains with areas ≥0.00045 mm² observed in thin section. A least-square linear fit of these data yields the constant used to determine apatite abundances by method *C*.

The database also includes analyses of questionable or poor quality within separate database tables. These tables, which have names beginning in *xx_* (e.g., Table 4), provide such data for three reasons.

1. Retention of all superceded data, some erroneous, allows uncertainties in petrographic analyses to be quantified.

2. Values that statistically are highly imprecise and unusable for individual samples, such as those for accessory minerals from point count, can be combined from several samples to provide averages with acceptable precision.

3. We reject some entire published datasets based on comparisons to a subset of higher accuracy. A more complete comparison might result in the acceptance of these data.

Accurate petrographic data can be used to resolve many geologic problems. For example, petrologic measurements can allow correct correlation and assignment of stratigraphic units within the stratigraphic column. Table 6 provides very simple statistics for abundances of selected minerals in units of the Wahmonie Formation that are shown in Figure 3, illustrating that the units are genetically related and are

a part of a single unique formation. Units of the Wahmonie Formation contain high plagioclase and biotite and low quartz and K-spar contents; such primary mineralogy readily distinguishes these units from nearly all others of the SWNVF. Units within the Wahmonie Formation are distinguished from each other by their abundances of individual mafic minerals.

Strat unit	n		Felsic phenocrysts				Mafic phenocrysts						Total %
			QZ	KF	PL		Biotite	Hbld	Opx	Cpx	Olivine		
Twu	5		0.02	0	23.68		8800	10900	41200	34400	0		33.23
Twm	7		0.04	0	21.34		14400	2210	38400	41500	10800		32.1
Twl	14		0.3	0	18.04		21000	19400	8720	0	0		23.25
Twlb	22		0	0	17.94		20300	14900	0	0	0		21.46
Tww	9		0.76	0.18	13.97		21700	572	466	23	0		17.18

Table 6. Simple statistical summary of abundances for selected primary minerals in units of the Wahmonie Formation. Abbreviations are QZ for quartz, KF for alkali feldspar, PL for plagioclase, Hbld for hornblende, Opx for orthopyroxene, and Cpx for clinopyroxene. Values are medians from *n* samples. Symbols for stratigraphic units are defined in database table *strat_list*. Felsic abundances are in volume percent, and mafic abundances are in parts per million by volume (ppmV). Includes only analyses entered into database by 23 October 1998.

Detailed Optical Mineralogy

Detailed information from optical mineralogy is provided for more than 1,000 petrographic thin section splits within database tables listed in Table 7. Both standard and detailed petrographic analyses provide abundances and a qualitative definition of alteration for each mineral, but only detailed petrographic analyses, described in the previous section, represent summaries derived from optical mineralogy of individual mineral grains. These optical mineralogic analyses provide supplemental quantitative or qualitative data for specific mineral grains including size, texture, alteration, and chemical compositions. During the process of detailed petrographic analysis, specific grains that require optical mineralogic analysis are identified on a photomap of a thin section (Figure 5). The identified grains, assigned unique grain IDs, may be a single crystal or consists of an assemblage of grain components (minerals), each identified by a unique grain component ID. Probe analysis (described in the next section) provides quantitative chemical analyses for grain component minerals. Complete mineralogic analyses provide data for a full or representative set of grains for each mineral, according to the method used for petrographic analysis. For example, the distribution of sizes (as the area in thin section) can be determined for each mineral determined by point count or method A. Appendix B provides examples of rules followed and uses for complete mineralogic analyses and Appendix C provides blank and completed forms for such analyses. Complete mineralogic analyses are available within the database for roughly 200 polished thin sections. Hardcopy information is available for approximately 600 additional sections from the senior author.

Table name	Description	Foreign key tables
ma_gr_measure	Grain component petrographic analyses	comp_list, pa_meth_list, ans_list, worker_list, qa_list
ma_gr_comp_texture	Grain component textures	texture_list
ma_clast_measure	Individual clast analyses	comp_list, pa_meth_list, strat_list, lith_list, worker_list, qa_list
ma_clast_alt	Clast alteration	alt_list
ma_clast_malt	Clast minor alteration	alt_list
xx_ma_gr_measure	Superceded or erroneous grain component petrographic analyses	comp_list, pa_meth_list, ans_list, worker_list, qa_list
xx_ma_clast_measure	Superceded or erroneous individual clast analyses	comp_list, pa_meth_list, strat_list, lith_list, worker_list, qa_list

Table 7. Database tables for detailed optical mineralogic analyses. Tables with names that begin *xx_* should not be employed for usual applications of mineralogic data.

Abundances of groundmass minerals cannot generally be determined within volcanic rocks of silicic affinity by optical methods. However, groundmass minerals of basic rocks are generally sufficiently coarse to quantify their abundances and 2-dimensional size ranges from point counts using reflected light. Basic volcanic rocks include basalt through andesite and their alkali-rich equivalents (Le Bas et al., 1986). Such rocks are also generally much simpler mineralogically than silicic volcanic rocks, and so fewer minerals are present, with abundances that usually provide satisfactory precision from point count. For basic rocks, complete mineralogic analysis usually provides 2-dimensional size ranges for all minerals except feldspar, which is generally so abundant that individual grains are bounded by other feldspar grains, rendering grain boundaries unrecognizable. Minerals that usually provide 2-D size distributions are olivine, clinopyroxene, and magnetite. Size distributions for each of these minerals, as well as for the largest feldspar grains, offer a more precise definition of basalt mineralogy than determination of separate abundances for "phenocryst", "microphenocryst", and "groundmass".

Minerals frequently occur within clasts in volcanic rocks. Clasts include:

Pyroclasts, such as pumices, shards, and lapilli of basalt or other cogenetic mafic components, representing original magma in most cases, and

lithics, which are foreign fragments of older rock.

Large clasts, clasts that contain more than a single component of interest, and clasts counted by point count are usually assigned a clast ID, and are described in the database (Table 7). Clasts generally become progressively less recognizable as alteration intensity increases. Mineral abundances from petrographic analyses include their occurrences within pyroclasts, but not within lithics. Aggregates of phenocryst-sized minerals, classified as lithics by some petrographers, are assigned *glomerophyric* textures and not considered lithics.

<u>Microprobe Analyses</u>

Quantitative mineral grain chemistry was obtained through more than 36,000 microprobe analyses, which provide more than 370,000 analyte concentrations for common minerals within database tables described in Table 8. This quantitative mineral chemistry can be related to quantitative and qualitative mineralogic determinations of the grain component, such as area in thin section or alteration. Multiple probe analyses may be available for any grain component. Typically, these replicate analyses represent different analytical locations, such as core or rim, within a single mineral grain component.

Table name	Description	Foreign key tables
probe_rep	Microprobe analysis description	probe_loc_list, qa_list, ref_list, topic_list, worker_list
probe_measure	Microprobe analyses	probe_standard_set_list, oxide_list
probe_end_members	Mineral end members	end_member_list
xx_probe_rep	Description for unacceptable microprobe analyses	probe_loc_list, qa_list, ref_list, topic_list, worker_list
xx_probe_measure	Unacceptable microprobe analyses	probe_standard_set_list, oxide_list
xx_probe_end_members	Mineral end members for unacceptable microprobe analyses	end_member_list

Table 8. Database tables for microprobe analyses. Tables with names that begin *xx_* should not be employed for usual applications of microprobe data.

The database also provides information from non-quantitative microprobe analyses. Most such analyses simply represent the recognition of a highly distinctive pattern of counts from energy dispersive spectroscopy (EDS) as shown in Figure 8. EDS analysis provides very accurate verifications of mineral identities that improve and validate the accuracy of petrographic analyses. Quantitative microprobe analysis is preferentially applied to a mineral with an uncertain identity, size large enough to allow significant zonation, unusual texture, or one intergrown with one or more other phase. EDS is generally used for grain components that are either unsuitable for quantitative analysis, or for minerals generally not analyzed. Detailed petrographic analyses incorporate either quantitative microprobe or EDS analyses for all grain components with identities that are even slightly uncertain.
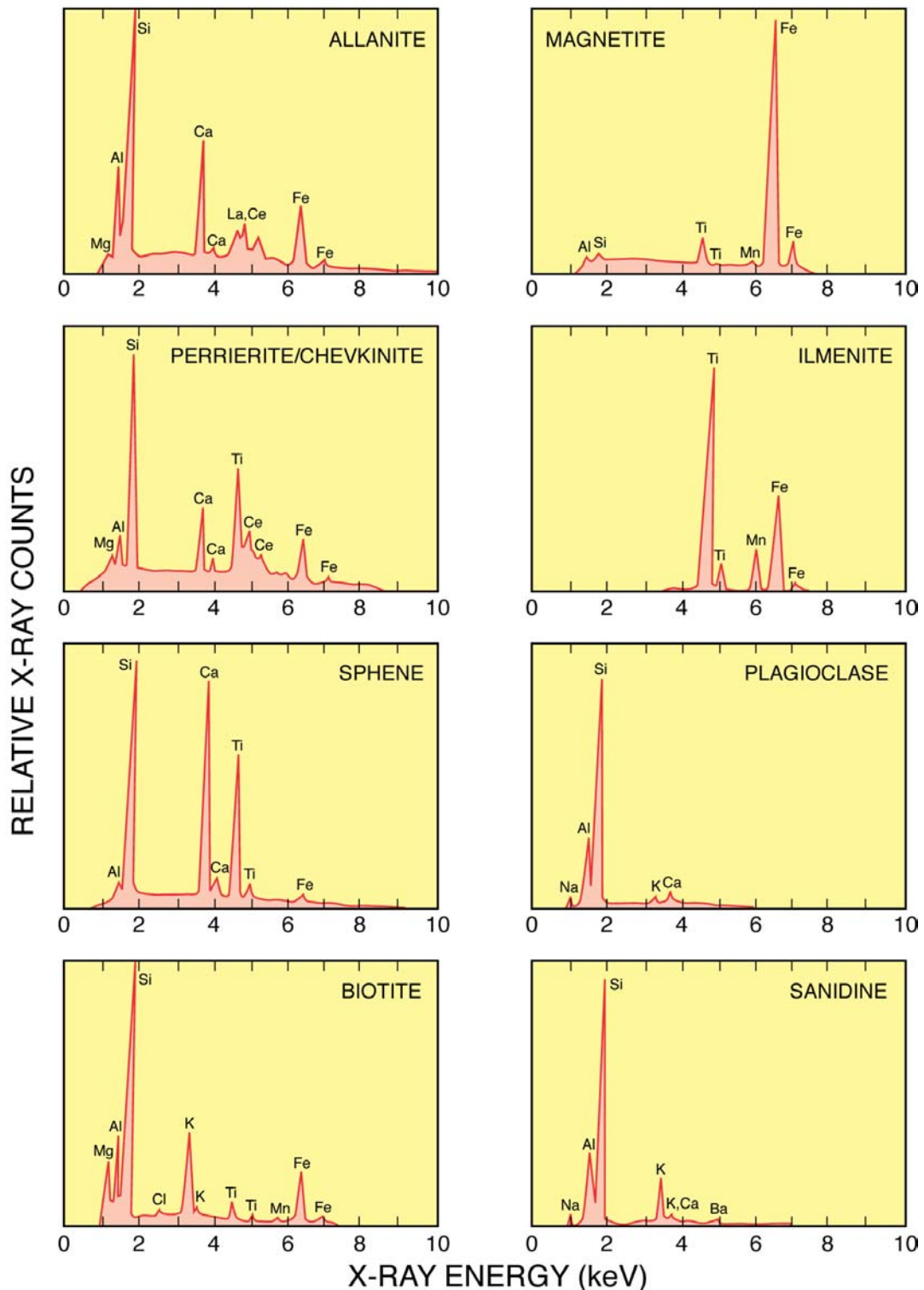
Figure 8. Energy dispersive spectra (EDS) for common minerals within volcanic rocks of the SWNVF.

The database also includes more than 3,000 unacceptable quantitative microprobe analyses within separate database tables that have names beginning in *xx_* (Table 8). Most of the unacceptable microprobe analyses do not meet acceptance criteria described in Table 9. Some published analyses meet

microprobe analyses do not meet acceptance criteria described in Table 9. Some published analyses meet the criteria, but the entire sets are considered unacceptable because a very large fraction of companion analyses, usually >30%, fail to meet the criteria of Table 9. The acceptance criteria have not yet been rigorously applied to all analyses, but only a few unacceptable analyses likely remain in the database. Database tables provide unacceptable analyses for the following reasons:

1. These analyses always provide valuable verification of optical mineralogy.

2. Universal standards of analytical quality are not presently applied for quantitative microprobe analyses, so many analyses deemed unacceptable might be acceptable to certain users of this database.

3. Most analyses are rejected owing to analytical problems with a small number of elements, usually a single element within a suite of about 10 analyzed; the remaining elements may offer very useful information.

Table 9. Acceptance criteria for microprobe analyses within this database (at end of document).

XRD Analyses

The database includes quantitative and semiquantitative analyses of mineral components by X-ray diffraction (XRD) for nearly 1100 samples within the database tables described in Table 10. These analyses provide the "whole-rock" mineralogy of each sample, although in some cases the sample may represent a separated mineral or component such as pumice. Mineralogic analyses by petrographic methods provide a complementary data set that represents only phenocryst minerals, which are large enough to be recognized by optical techniques. Phenocrysts form within the magma prior to each volcanic eruption, and comprise a small fraction of the sample, typically between 0 to 30% of the rock. This assemblage of phenocrysts and their chemistry are almost always distinctive for each volcanic unit. Thus, petrographic analyses define mineralogy applicable to stratigraphy. Glass or tiny secondary minerals, which define mineralogy applicable to alteration, and which comprise the remaining 70 to 100% of most volcanic rocks, are difficult or impossible to quantify by petrographic methods. The large fraction of secondary minerals dominates the results of whole-rock sample analyses. Thus XRD analyses are most suitable for defining mineralogy applicable to alteration. Knowledge of the XRD method used, and of the nature of the sample are key considerations in the successful evaluation of these data.

XRD measurements are reported in the database as units of weight, whereas petrographic measurements are in units of volume. To exactly relate the two measurements requires knowledge of the bulk density of the sample, as well as the density of each constituent mineral. Non-numerical abundance measurements originally reported, e.g. "not detected", "trace", have been converted to numerical values recommended or implied by the analysts. Reports of "not detected" are represented in the database as zero. "Trace" abundances are typically assigned a value of 0.5% or 0.25%, which is assumed to represent the two-sigma uncertainty.

Table name	Description	Foreign key tables
xrd_split	Method for XRD analysis	xrd_meth_list
xrd_measure	XRD analyses	comp_list

Table 10. Database tables for X-ray diffraction (XRD) mineralogic analyses.

This first revision of the database excludes the large set of XRD analyses within the GEODES database (Winterkamp et al., 1985). However, we anticipate adding these and many additional XRD analyses within the next version.

Geologic Intervals from drillholes

Database tables described in Table 11 define stratigraphic units, lithologies, major and minor alterations, and fracture and lithophysal zone intensities within elevation (depth) intervals for more than 750 drill holes of the SWNVF. These characteristics of the rock column, defined independently within successive intervals of elevation, are together termed "geologic intervals". The geologic intervals very strongly relate to the chemical, mineralogic, petrographic, and physical characteristics of the rock column provided by sample splits at points within geologic intervals, and to geophysical logs. Geologic intervals can be combined with these data to develop three-dimensional representations of the chemical, mineralogic, and petrographic characteristics of the subsurface, as well its physical properties.

Table name	Description	Foreign key tables
strat_int	Stratigraphic intervals	strat_list
lith_int	Lithologic intervals	lith_list
alt_int	Alteration and minor alteration intervals	alt_list, topic_list
frac_physae_int	Fracture and lithophysal intervals	frac_physae_list, topic_list
geol_int_ref	Citations for geologic interval characteristics	topic_list, ref_list

Table 11. Database tables for geologic intervals from drillholes.

Geophysical Logs

This first revision of the database has added more than 21 million records that represent all geophysical logs originally within the GEODES database (Winterkamp et al., 1985). A large variety of geophysical logs added include density, porosity, water content, spectral gamma (K, U, Th), caliper, gravity, and many others listed within foreign key table *log_type_list*. Nearly all of these logs represent drill holes within Los Alamos use areas of the NTS, which occupy the southern half of Yucca Flat and the eastern part of Pahute Mesa. We have removed nearly 80,000 records transformed from GEODES that represent inferior or erroneous portions of geophysical logs, or entire logs. Most of these records reside within the database table *geophys_int;* the records removed reside within database table *xx_geophys_int,* both described in Table 12. The process to remove inferior or erroneous portions of geophysical logs is presently incomplete but should be complete with the next revision of the database.

Table name	Description	Foreign key tables
drill_hole_info	Drill hole information	12 lists, described in table_desc
drill_fluid	Drilling fluid	drill_hole_list, hole_fluid_list
hole_gen_info	Miscellaneous information for drill holes	drill_hole_list, hole_geninfo_list
hole_log_info	Description of each geophysical log	drill_hole_list, log_type_list, worker_list, format_list
log_fluid	Fluids within hole during geophysical logging	hole_log_info, hole_fluid_list
log_constants	Constants used to compute geophysical log	hole_log_info, log_type_list, log_constant_list
log_calib_consta nts	Constants used to calibrate geophysical log	hole_log_info, log_type_list, log_constant_list
log_worker	Geophysical logger	hole_log_info, topic_list, worker_list
geophys_int	Geophysical logs	location, log_type_list
xx_geophys_int	Geophysical logs of unacceptable quality	location, log_type_list

Table 12. Database tables for geophysical logs from GEODES.

Physical Properties

This first revision of the database contains no tables for physical properties. However, we anticipate adding database tables within the next revision of the database to further incorporate the GEODES database (Winterkamp et al., 1985). Physical properties represented within GEODES include grain density and sample density, mostly for samples within Los Alamos use areas of the NTS.

III. DATABASE OBJECTS AND STRUCTURE

The database is a collection of visual (field) and laboratory measurements as well as supporting metadata, taken for samples from geographic points or for depth intervals from field observations or geophysical logs within the SWNVF. Field measurements include such items as color, alteration, and texture. Laboratory measurements include various kinds of chemical analyses, age determinations, X-ray diffraction analyses, petrographic analyses, including optical mineralogic analyses for individual minerals, microprobe analyses, and physical properties such as grain and bulk densities. The database is structured so that subsets of information can be extracted for specific geographic and time (age or stratigraphic) points or ranges. The database is designed to facilitate comprehensive, integrated analyses of all available geologic data from the SWNVF. Most important types of geologic information are included within the initial version of the database or work is in progress to add such information to an updated version. A few types of data important for geologic interpretation are omitted from this database; prominent among such missing information is paleomagnetic data (see, for example Hudson et al., 1994).

Relational Databases

A relational database consists of a set of tables. These tables have a row/column structure in which columns reflect "entities" or data items and associated attribute information, while rows reflect observations of the entities and associated attributes. Entities can be simple, i.e. location (loc_id), sample (sam_id) and split (spl_id); or complex, i.e. *split_id/run_no*. Attributes provide descriptive and/or

auxiliary information which "track" with the entity to create a unique record or observation. Examples of attributes are north and east coordinates, sample type, worker(s), weight % SiO_2, or volume % quartz.

If there is a need to extract specific observations from a database table, then the entity "identifier" must be unique, non-null and thus distinguishable from all other entity entries in the table. For example, if the results (attributes) from each of several analytical runs for a *split_id* need to uniquely identified, the initial entity: *split_id*, may need to be combined with an attribute: *run_no*, to create a unique, multi-column entity identifier, defined as a Primary Key. The Primary Key of a table, composed of a single or multiple columns, provides an unambiguous link to auxiliary tables, and is considered as a Foreign Key by the auxiliary tables. For example, the set of attribute information from a single sample may reflect the efforts of several workers (see Figure 9). A spreadsheet-type approach to this case would be either to have columns: worker_#1, worker_#2 ... in a single observation or row of the spreadsheet/table, or to have multiple rows, with the only difference between rows being the name of the worker. The relational database approach would be to define the *sam_id* as the Primary Key, and drop the worker field/column from the initial table so that all observations maintain a one-to-one relationship between attributes and entities. The worker information, which reflects a one-to-many, worker-to-sample relationship, would be stored in a separate table with columns: *sam_id*, *worker_name*. *Sam_id* would be defined as a foreign key, referencing the *sam_id* column of the initial sample table. This approach obviates the need for creating multiple, near duplicate columns in a table, or creating rows of mostly-redundant information, yet allows full recovery of all of the data associated with the entity. The process of minimizing redundant data within the database is called normalization.

Table A.

Sam_id	attr #1	attr #2	attr #3	worker #1	worker #2	worker #3
BV-3	12.3	6.4	blue	Smith	Jones	Barney
BV-4	8.2	2.3	grey	Jones	Barney	

Table B.

Sam_id	attr #1	attr #2	attr #3	worker
BV-3	12.3	6.4	blue	Smith
BV-3	12.3	6.4	blue	Jones
BV-3	12.3	6.4	blue	Barney
BV-4	8.2	2.3	grey	Jones
BV-4	8.2	2.3	grey	Barney

Table C.

Sam_id	attr #1	attr #2	attr #3
BV-3	12.3	6.4	blue
BV-4	8.2	2.3	grey

Table D.

sam_id	worker
BV-3	Smith
BV-3	Jones
BV-3	Barney
BV-4	Jones
BV-4	Barney

Figure 9. Comparison of spreadsheet and relational table structures. Spreadsheet Table A has multiple columns for workers. Identification of work performed by Barney would require a query of three fields. Spreadsheet Table B has a single worker field, but must duplicate other attribute data within each row. Relational Table C stores unique (one-to-one) attribute values for a sam-id, while relational Table D

stores multivalued (one-to-many) values for a *sam-id* (primary key). A query of the worker field of Table D, with a relate to Table C by *sam-id*, could retrieve all attribute data (attr #1, attr #2, attr #3) created by Barney.

<u>Database for the SWNVF</u>

The database for the SWNVF is relational, and is currently loaded in the commercial Oracle relational database management system (RDBMS) product. Data objects and structures (outlined in Figure 10) were created to support full extraction of all information originally contained within nonrelational database tables, ensure extensibility of the data set, establish hierarchical, parent-child relationships, and allow geographically-based data retrieval. The database was "normalized" to reduce storage of redundant data, allow enforcement of quality assurance (integrity) during the database loading stage, and fully exploit relationships among the data. Finally, accelerated storage retrieval has been initiated to a small degree through de-"normalization", which provides repetitive data within two or more tables to avoid frequent linking between the tables.
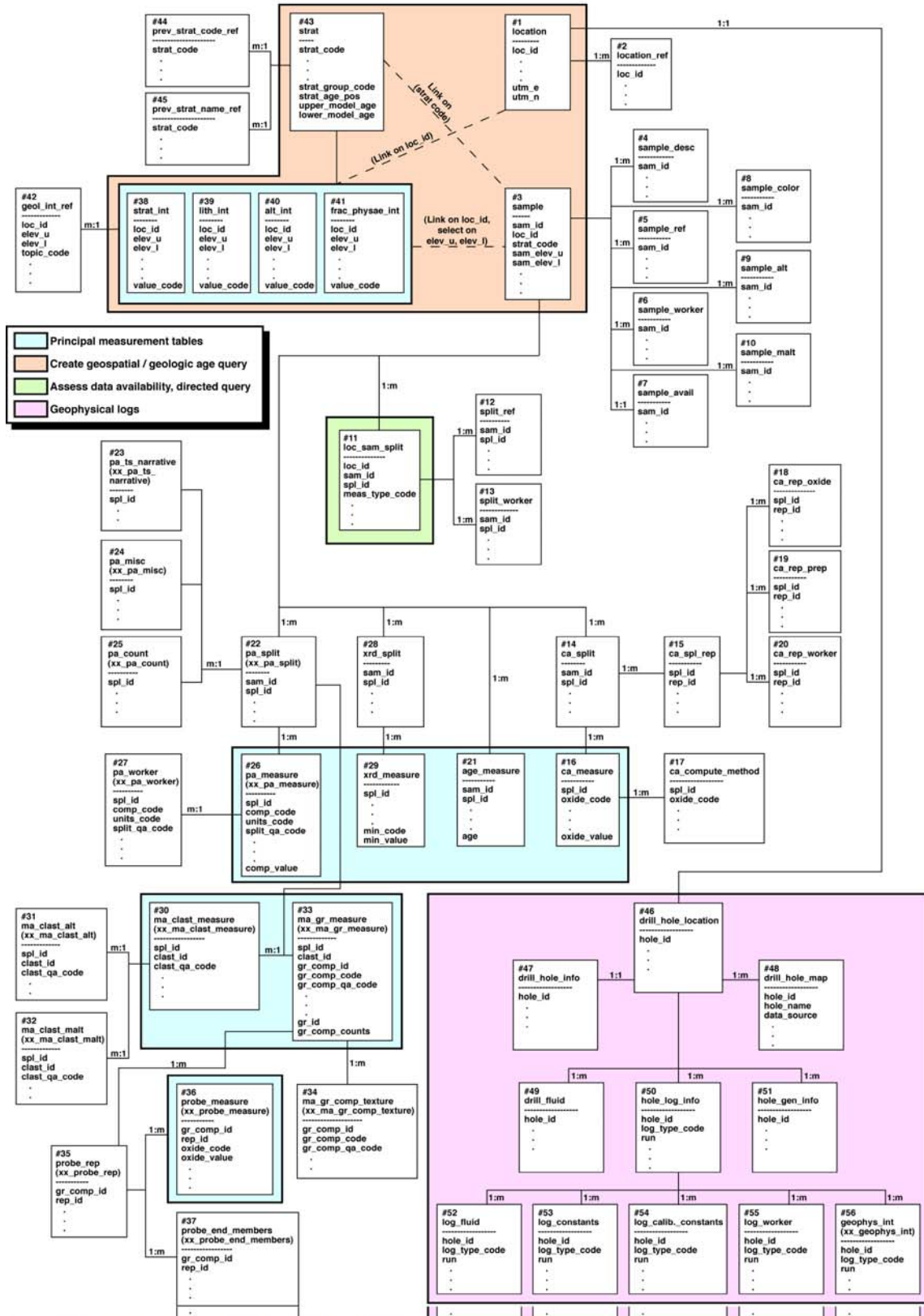
Figure 10. Entity-relationship diagram for geological data of the SWNVF

The entity-relationship model for "point" data results in a set of database tables that also incorporate the integral hierarchy at which these data were collected. This hierarchy is reflected through successive one-to-many tables in which:

- a location (x, y coordinate) can have many samples (with different z coordinates),

- a sample can have many splits (i.e. chemical, petrologic),

- a split can have many measurements (i.e. chemical - Na, K, Mg) and,

- measurements can have replicates (although measurements averaged from replicates are reported in the database, except for microprobe analyses where mineral zonation can be a factor).

Database tables that define location, sample, and split (i.e. *pa_split*, *ca_split*, *ma_split*) contain columns that define attributes specific to the location, sample, or split. These tables also provide cumulative supporting information for measurements. Additional descriptive information for each measurement such as uncertainties, units of measurement, etc. apply directly (uniquely) to a particular measurement and are usually contained in tables at the measurement level. At all levels, one-to-many relationships between data fields (entities) within the data relevant at that level are managed by placing these data in separate tables.

The entity-relationship model for data from geologic intervals is simpler than that from single points. Geologic intervals normally represent several types of observations for each drill hole, each observation represented by a character string. Measurements of all types are combined within a single large database table; an attribute identifies the measurement type for each geologic interval. The *loc_id*s that provide drill hole names, together with depths/elevations of the interval boundaries, allow data for geologic intervals to be integrated with data for samples. Because there are no "splits" for geologic intervals, fewer data are required to define attributes.

At present, measurement tables contain metadata (information about the data) as well as measurements. These tables could be split into pairs of "clustered" tables although it may be difficult in some cases to discriminate between data and metadata. For example, measurement units might be viewed as data critical to the measurement, or simply might represent an attribute to be stored in a separate table.

Foreign Key Tables

Foreign Key tables provide data code definitions, subsidiary data code information, acceptable values for fields (to insure data retrievability), and/or groupings of data.

Many of the primary tables contain descriptive data that are abbreviated as codes. Foreign Key tables with the naming convention "attribute"_list can be linked to the primary tables to insure that input data is correct, and to allow expansion of the codes at the time of data retrieval, as shown in Table 13.

texture_code	texture_name
A	partly altered
B	blackened mafic
G	granular
H	shreddy (disaggregated)
M	microlite or groundmass phase
P	prismatic (elongate)
S	shattered
W	wormy (coarse) resorption

Table 13. Portion of the Foreign Key table *texture_list*

The Foreign Key tables allow compaction of the data in the larger primary tables and can also supply additional subsidiary information about the data item. For example, worker names are generally entered as initials. The database table *worker_list* contains the worker code **and** the worker name, organization, city, and state. Other tables, such as *oxide_list*, contain information to allow mapping and/or data conversion, as shown in Table 14.

oxide_code	oxide_name	element_code	element_name	ox_el_wt_ratio
Ag2O	Silver Oxide	Ag	Silver	1.07416
Al2O3	Alumina	Al	Aluminum	1.88988
As2O3	Arsenic Oxide	As	Arsenic	1.32038

Table 14. Portion of the Foreign Key table *oxide_list*

Database table *ca_measure* provides all chemical analyses in the database as their most common oxide, except for elements that generally occur in native form, such as mercury. The last field (*ox_el_wt_ratio*) in table *oxide_list* provides the conversion factor from oxide weight to element weight, which allows extraction of chemical analyses in elemental representation.

Hierarchical groupings for codes is accomplished by imbedding a parent:child relationship within a Foreign Key table. Within such tables, paired fields containing the same type data represent the "parent" and "child", as illustrated in Table 15.

Column 1	Column 2	Column 3	Column 4
record ID	*child*	*parent*	*other data fields*
1	C	B	
2	D	B	
3	B	A	
4	A		

Table 15. Illustration of parent:child relationships within database

implying the hierarchical grouping

```
        A
        |
        B
       / \
      C   D
```
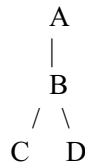
Use of such a Foreign Key table allows extraction of other data fields based on a "parent", all "children", the children's "children", etc. to some specified level. Thus, in the example above, data fields can be extracted for all records where Column 2 is B, C, or D by extracting records where Column 3 is B, that is, extracting records for B and its children. In this normalized database, parent:child relationships are defined within a Foreign Key table and not by an additional column within a data table. An example within the database is Foreign Key table *comp_list*, which defines components, mostly minerals, that are analyzed by petrography and by XRD, as shown in Table 16.

comp_code	*comp_name*	*comp_group_code*
child		**Parent**
WW	all minerals	(no parent)
FE	felsic minerals	WW
FS	Feldspar	FE
KF	K-spar	FS
PL	Plagioclase	FS
QZ	Quartz	FE
AO	Anorthoclase	KF
MC	Microcline	KF
OR	Orthoclase	KF
SD	Sanidine	KF

Table 16. Portion of the Foreign Key table *comp_list*

One could use this table to create a query that would extract measurements for all felsic minerals (FE, FS, KF, PL, QZ, AO, MC, OR, SD) through identification of the parent component (FE). The hierarchy also allows use of felsic mineral abundances in special cases. For example, feldspar is often completely destroyed by hydrothermal alteration, rendering K-spar and plagioclase indistinguishable and thus individually indeterminate. In such cases, total feldspar might be determined for comparison with total feldspar in samples outside the hydrothermally altered area. Another example is to combine individual analyses determined by a petrographer when these are demonstrated to be inaccurate. In many cases optical petrographic analyses are erroneous for K-spar and plagioclase. Combining these into total feldspar retains reliable petrographic information while avoiding a complete loss of information. The hierarchy established in database table *comp_list* for mafic minerals has particularly useful application in petrographic analysis owing to the great sensitivity of these minerals to alteration.

Overlapping groupings of codes can be accomplished by a many-to-many mapping of codes. The mapping table *lith_group_map* can be combined with the Foreign Key table *lith_list* to allow groupings of lithologic information to be extracted from primary tables. Portions of the tables *lith_group_map* and *lith_list* shown in Tables 17 and 18 illustrate how a particular lithology can be included within two or more groups. For example, an extraction of information for dikes should include basaltic dikes (*lith_code BD* in Table 17), but an extraction for basic rocks should also include basaltic dikes. This is

accomplished by defining two parents for *lith_code BD* in Table 18, assuring retrieval from any appropriate parent.

lith_code	lith_name
BA	basic rocks
BD	basaltic dike
BS	basalt
GB	gabbro
ID	dike
IS	shallow intrusives
IN	intrusive

Table 17. Portion of the Foreign Key table *lith_list*

lith_code	lith_group_code
BD	IN
BD	BA
BS	BA
GB	BA
ID	IN
IS	IN

Table 18. Portion of the Foreign Key table *lith_ group_map*

IV.   APPLICATIONS OF THE DATABASE

This database is designed for a wide variety of applications by a wide variety of users. To guide users who may be unfamiliar with petrographic, mineralogic, and chemical data, we provide a few examples of the past application of data now within this database.

Volcanic eruptions are often complex, and the eruption of a single magma can result in a variety of rock types, or lithologies. An example is rhyolite of Echo Peak (stratigraphic symbol *Tpe*). This stratigraphic unit represents magma erupted 12.7 million years ago. Like many rhyolites, the ascending magma contained large amounts of volatile components, mostly water. Sudden outgassing from the top of the magma produced an eruptive column of ash that fell to form an initial deposit of bedded tuff. As the eruption progressed, perhaps in several stages, continued outgassing depleted later-erupted magma in volatiles, and eventually lava was erupted. This lava flowed over the bedded tuff, fusing the uppermost portion into a welded tuff. This eruptive history was first recognized by Byers et al. (1976a) from petrographic analyses of the different lithologies (Figure 11). The three constituent lithologies of rhyolite of Echo Peak are very different in appearance and physical character, and during field mapping, these lithologies were each assumed to represent a different stratigraphic unit. The welded tuff was initially thought to represent ash flow of the Pah Canyon Tuff.
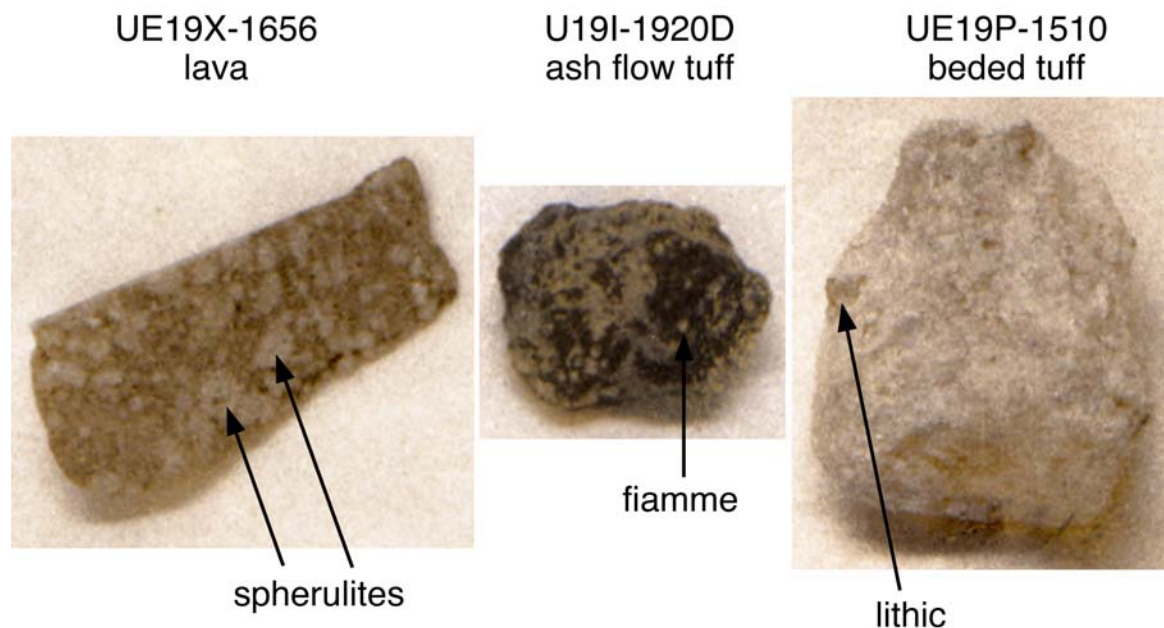
Figure 11. Photo shows three very different lithologies from rhyolite of Echo Peak, all produced from the same magma. Their intimate relationship was uncovered using the petrographic, chemical, and mineral chemical data in this database. Volcanic lithologies are often very complex, and the relationship between adjacent exposures of volcanic rock frequently cannot be determined using field methods.

Subsequent application of mineral chemical analyses by electron microprobe has proven the common parentage for the three different lithologies from rhyolite of Echo Peak (Figure 12). In combination with detailed petrographic analyses, microprobe analyses have further demonstrated that rhyolite of Echo Peak was erupted across a large area. This unit occurs at Pahute Mesa, mapped as pyroxene-bearing flows by Byers and Cummings (1967), and also at the northern end of Yucca Mountain, some 30 km to the south (see Figure 1 for locations), where it was named rhyolite flow by Christiansen and Lipman (1965). The equivalency of these volcanic units cannot be established by field geology, because the distance between these locations is completely covered by younger rocks related to the Timber Mountain caldera.
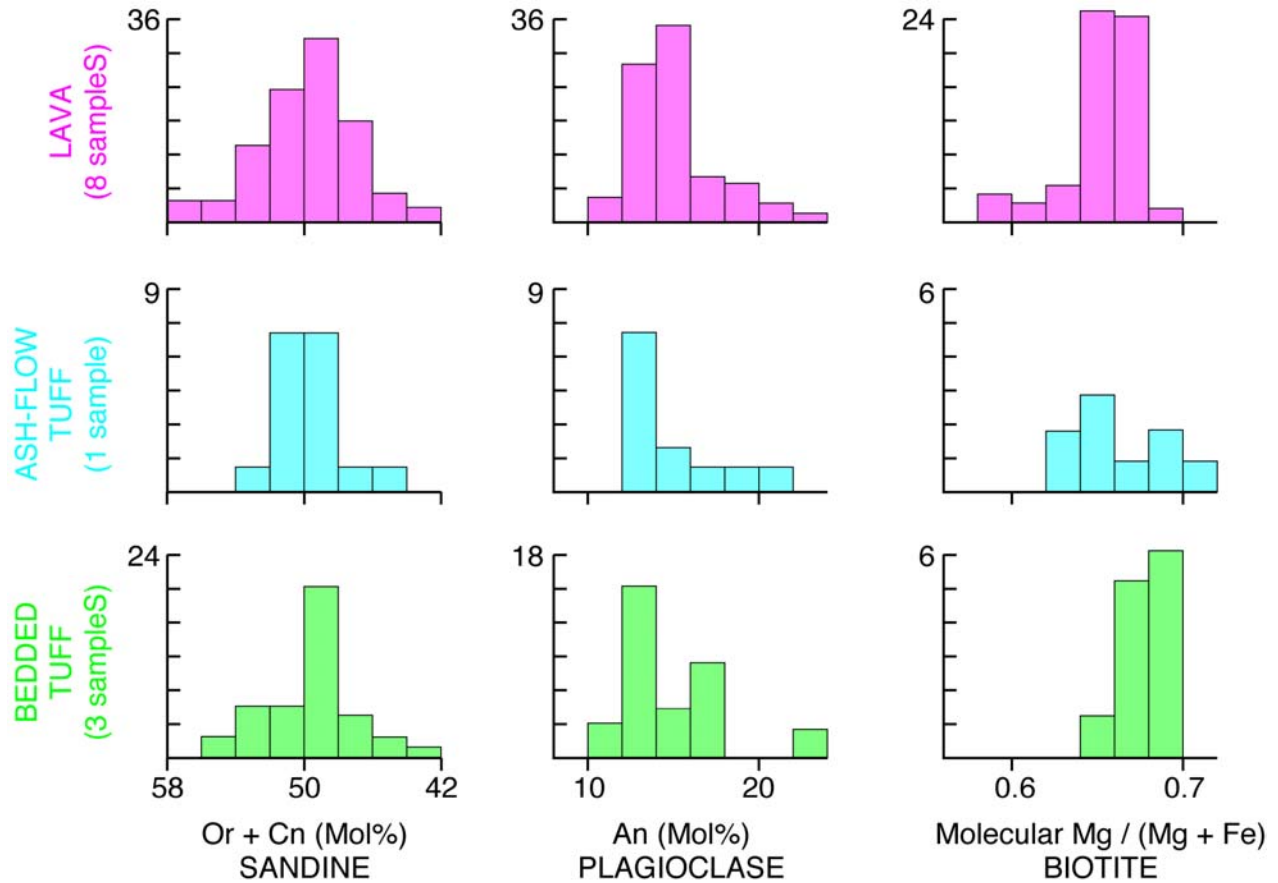
Figure 12. Histograms of mineral chemical analyses by electron microprobe for the three different lithologies from rhyolite of Echo Peak. These analyses support the common magmatic parentage inferred from petrographic analyses for the three very different lithologies of Figure 11.

The application of petrographic analyses and mineral chemical analyses has demonstrated the widespread equivalence of older volcanic units within the SWNVF that were previously unrelated. Figure 13 shows the location of two major volcanic units on opposite sides of the Timber Mountain caldera that were derived from the same magma, and Figure 14 shows the stratigraphic column that was correlated on the basis of petrography and microprobe analyses (Warren, 1983b).
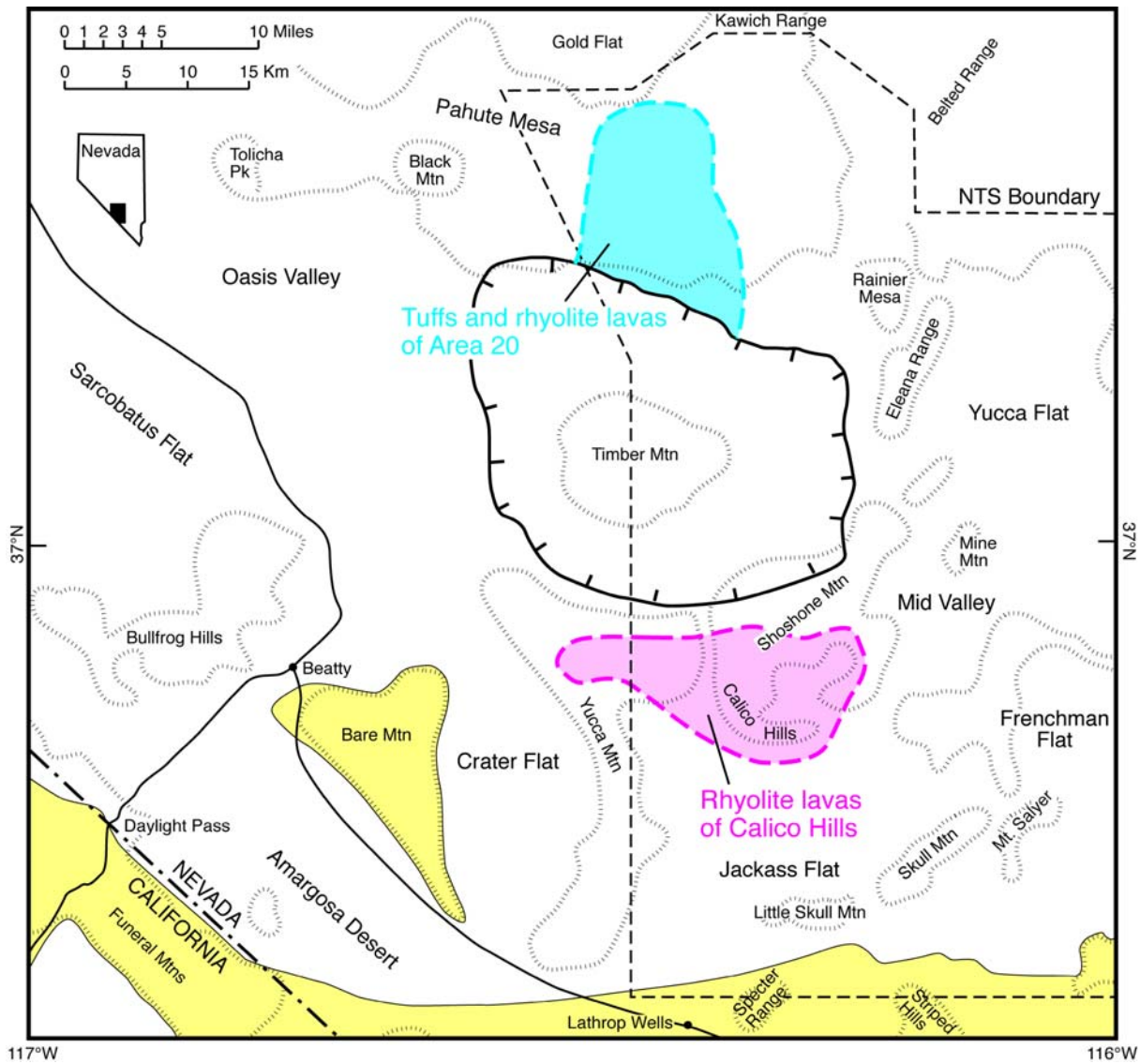
Figure 13. Location of tuffs and rhyolite lavas of Area 20 within Pahute Mesa region and rhyolite lavas of Calico Hills within Yucca Mountain region. These units are separated by the younger Timber Mountain caldera, and so cannot be correlated by field geologic methods. The application of petrographic analyses and mineral chemical analyses by Warren (1983b) demonstrated the magmatic equivalence of these two major units, now named the Calico Hills Formation. Volcanic rocks are absent within areas shaded yellow.
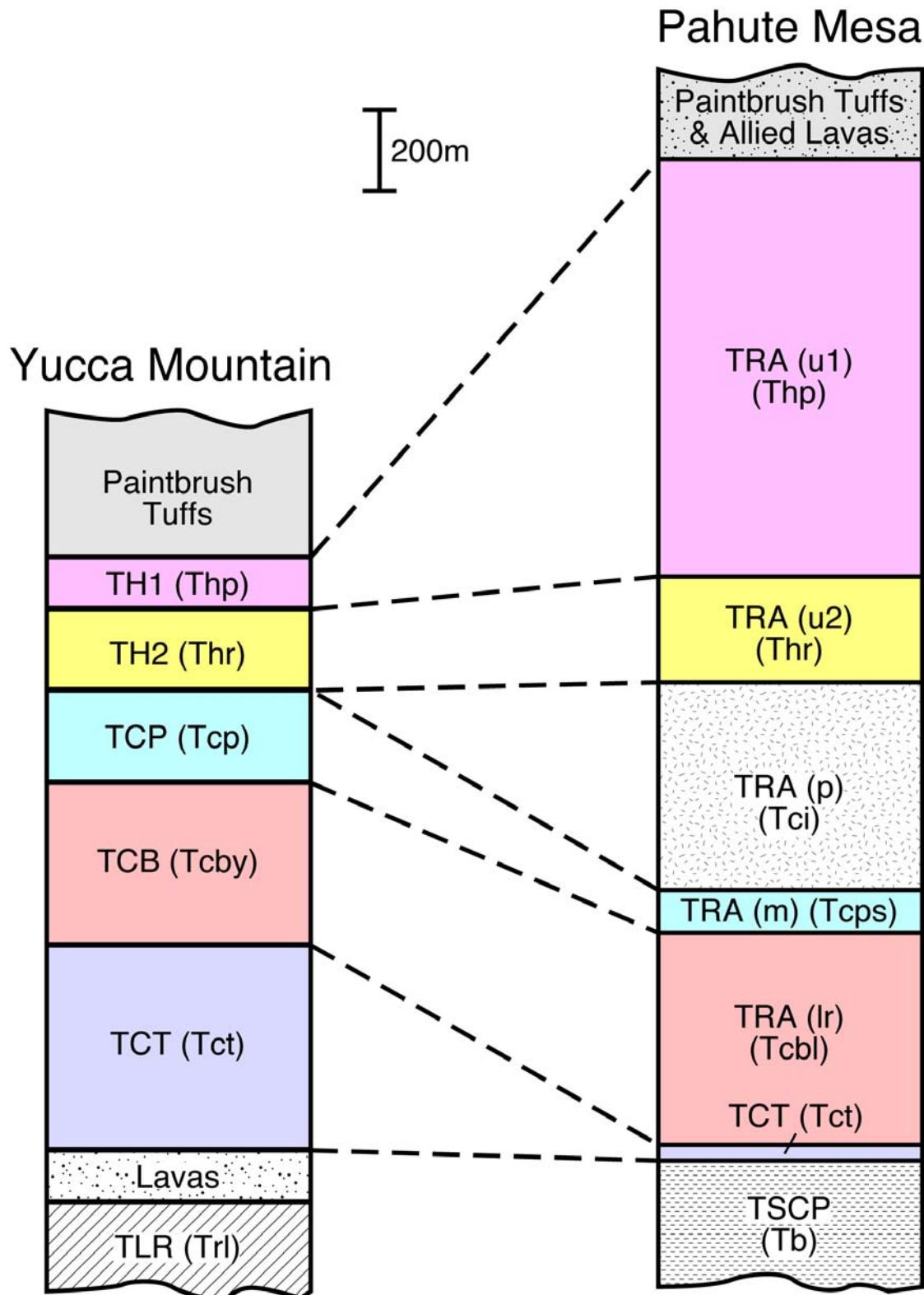
Figure 14. Correlation of stratigraphic units between the Pahute Mesa and Yucca Mountain regions, based on petrographic analyses and mineral chemical analyses by Warren (1983b). Symbols are for petrologic zones defined in the original paper; parenthetical symbols are those presently used for stratigraphic units in the database.

Petrographic analyses and mineral chemical analyses have also solved critical problems where two different stratigraphic units have identical field characteristics, and were miscorrelated. On the south face of Pahute Mesa, nonwelded ash flow tuffs occur beneath Tiva Canyon Tuff on opposite sides of the Scrugham Peak fault. This tuff was well characterized east of the fault as a very quartz-rich unit, the tuff of Blacktop Buttes. Petrographic analyses and mineral chemical analyses (Figure 15) demonstrated that exposures on opposite sides of the fault represent two very different units (Warren et al., 1985). This single miscorrelation prevented regional correlation of units within the lower half of the stratigraphic column of the SWNVF. The correct stratigraphic assignment for ash flows on opposite sides of the fault also demonstrated that the Scrugham Peak fault was active during at least two different episodes, establishing an important feature of tectonism within the volcanic field.
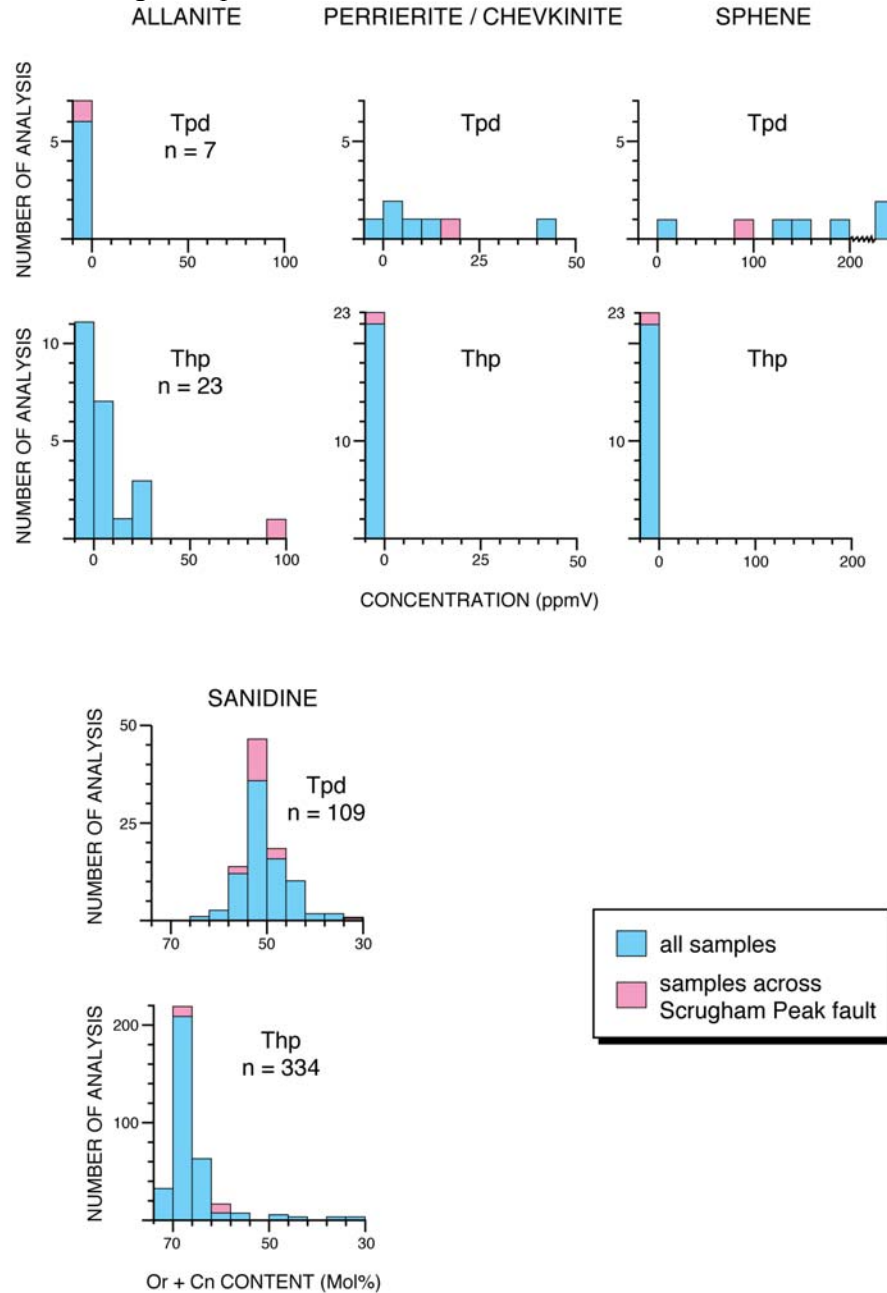
Figure 15. Histograms that illustrate use of petrographic and mineral chemical data to demonstrate that two exposures of nonwelded tuff with indistinguishable field characters are different units (Warren et al.,

1985). Nonwelded tuff east of the Scrugham Peak fault, mapped as tuff of Blacktop Buttes, is mafic-poor Calico Hills Formation (Thp). Nonwelded tuff west of the fault is rhyolite of Delirium Canyon (Tpd). Cross-hatched patterns represent reference samples from each unit, whereas shaded patterns represent samples of nonwelded tuff that had been miscorrelated across the fault.

Petrographic, mineralogic, and chemical data within this database were initially applied to solve stratigraphic problems. These data have been well applied for this purpose, resulting in a robust characterization of the stratigraphic column (Figure 16). However, other applications of these same data are possible, including statistical analyses to define relationships among petrographic, mineralogic, and chemical data, and spatial relationships for each type of data. The possible applications of this database are many. Our primary goal in designing and publishing this database is to provide this information in a form that is easy to apply.
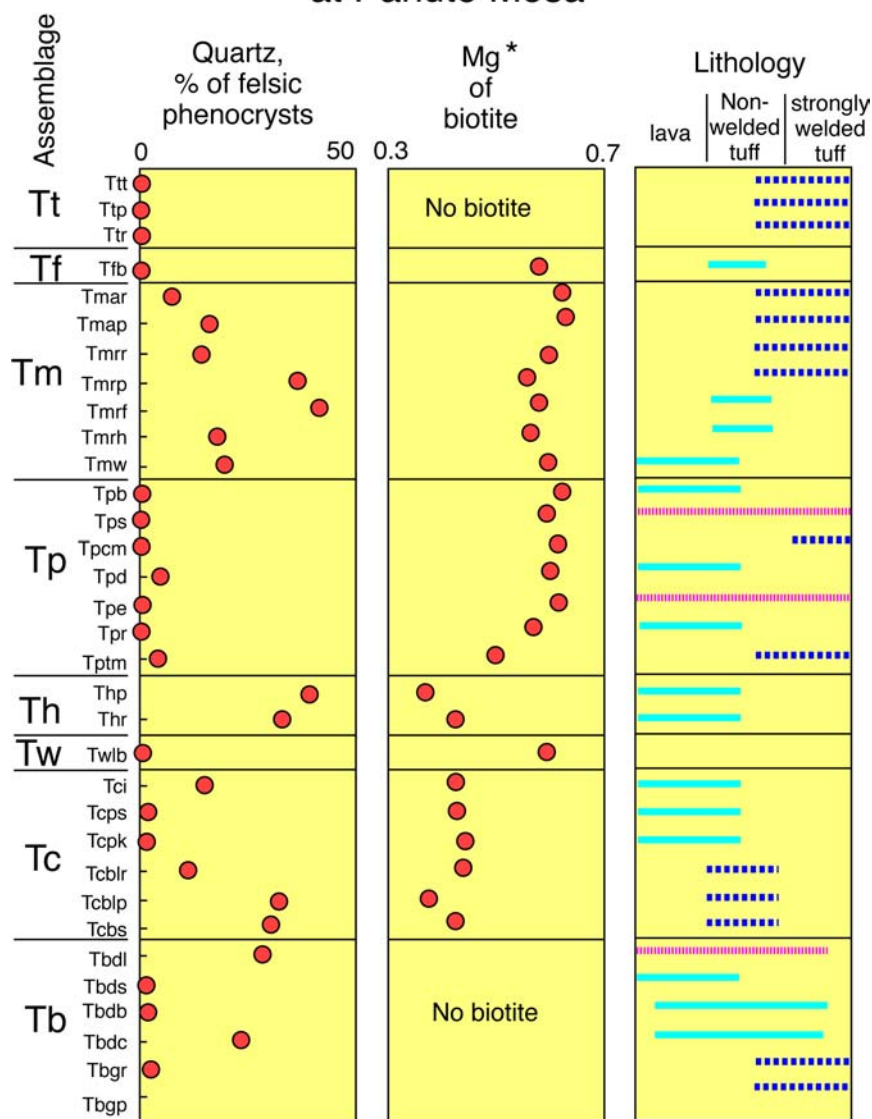
Figure 16.   Selected petrographic, mineral chemical, and lithological analyses for some of the stratigraphic units within the SWNVF. The more than 300 volcanic units, for example Ttt, reside within volcanic assemblages such as Tt.   Assemblages consist of a group of units that display similar

petrographic, mineral chemical, and lithologic character. Parent-child relationships imbedded in the stratigraphic table allow easy extraction of data for related groups of stratigraphic units.

V. ACKNOWLEDGMENTS

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Appendix A. Development and evolution of containment science activities for the Nevada Test Site at Los Alamos National Laboratory

The science of Containment integrates nuclear and conventional physics, explosion phenomenology, geologic knowledge, and past testing experience to ensure the safest conduct of nuclear tests (Brownlee, 1983; Brownlee, 1993). Separate Containment programs at LANL and at LLNL served to provide effective review of the prospectus for each proposed test, and the USGS served to provide specific review for geologic work within both programs, as well as to provide relevant research. Final approval of the Containment plan for each test was issued by the Containment Evaluation Panel, a committee of experts within each of the disciplines that constitute the science of Containment (Carothers, 1993).

At Los Alamos, Rick Warren began petrographic analyses in late 1980, initially to support the Yucca Mountain project, then in early 1981 to improve geologic characterization for containment of tests at Pahute Mesa. His work was inspired by the petrographic work of Frank Byers, initiated during the mid-1970's to support field mapping and Containment for the USGS. Frank's petrographic analyses, summarized in Byers et al., (1976a), demonstrated the powerful applicability of accurate, quantitative (modal) petrographic analysis to geologic problems within the SWNVF. Frank's analyses are based on extraordinarily large total counts (see Quinlivan and Byers, 1977 for examples), and coupled with his extensive experience and skill, provide exceptionally accurate analyses for major and minor constituents. Warren et al. (1984) demonstrated that accurate mineral chemistry and mineral identifications obtained by electron microprobe provided additional, equally powerful data to solve geologic problems. Warren has carried out a concerted campaign to characterize the mineralogy and mineral chemistry of all volcanic units within the SWNVF, particularly between 1980 and 1987. During the first year of this campaign, he developed techniques for the precise determination of minor and trace constituents (Warren et al., 1984; Warren et al., 1989b). Byers et al. (1976a) demonstrated that minor and trace constituents are very important petrographic data, but quantification of trace constituents had never before been attempted for routine optical analysis. The techniques for precise determination of minor and trace constituents require comprehensive documentation, and provide an extremely high level of quality assurance for petrographic analysis as an additional benefit.

The application of Warren's work resulted in the solution of several regional geologic problems concerning the SWNVF (Warren, 1983b). By the late 1980's, he was collaborating with David Sawyer and his colleagues of the Containment Research Group of the USGS, led by Paul P. Orkild, to address regional geologic problems within the volcanic field. With Sawyer and his colleagues contributing field work, age dates, and expertise in stratigraphy, an improved system of stratigraphy was developed for the SWNVF (Warren et al, 1989a), both formally for major units (Sawyer et al., 1994) and informally for all units (Ferguson et al., 1994).

During 1984, Sue Freeman began assembly of geological data into a non-relational database to improve its applicability to both Containment and regional geologic problems (Freeman et al., 1985). In 1987, Emily Kluk helped Rick to resume this effort, using commercial data storage and analysis software. Beginning in 1995, Greg Cole has transformed and reorganized the original electronic dataset into a widely accepted, standard form that allows widespread use of these geologic data for future Containment needs or for a variety of other possible applications.

Appendix B. Examples from complete mineralogic analysis of sample BH86N/33 and their application in detailed petrographic analysis

Anorthoclase was determined by point count from petrographic analysis of split BH86N/33(B. Within Appendix C are the form used to document methods of petrographic analysis as well as the completed form for split BH86N/33(B. Other splits identified in table *loc_sam_split* provide petrographic data from a glass covered thin section, an age date, and chemical analyses by both neutron activation analysis and by X-ray fluorescence. From table *ma_gr_measure*, four grains that contain anorthoclase (*gr_comp_code* equals *AO*) were intersected by the point count, and therefore represent this mineral within split *B*.   The grain with a *gr_ID* of *27* consists entirely of anorthoclase, but grains *33* and *43* are intergrown with sanidine. Within Appendix C are the form used to document optical analysis for individual grains, as well as a single page of the completed form for split BH86N/33(B. Grain *57* has an area of .0178 mm^2, and is intergrown with plagioclase that has an area of .0805 mm^2. Whole counts are assigned to each particular grain for each mineral group of felsic, mafic, and Fe-Ti oxide minerals, as defined in database table *comp_list*. Counts for individual members of each group are apportioned fractional counts based on their relative areas, so anorthoclase *57* is assigned 0.18 counts and plagioclase *57* is assigned 0.82 counts. Using each *gr_comp_ID*, table *ma_gr_comp_texture* reveals that plagioclase *57* is *wormy*, or coarsely resorbed, whereas anorthoclase *57* has no unusual texture. Table *ma_gr_measure* reveals that energy dispersive and quantitative electron microprobe analyses are available for both anorthoclase and plagioclase *57*, as described in the microprobe section.

With one exception, all intergrown grain components are described for each *gr_ID* represented in database table *ma_gr_measure*, regardless of the method specified for the mineral in table *pa_measure*. Only grain components >0.00045 mm^2 are always represented where a *grain count*, method *C* in database table *pa_method*, is applied; grain components ≤0.00045 mm^2 are represented only when they are the largest for a grain. No phases other than felsic minerals are assigned the same *gr_ID* as grains that contain anorthoclase, so no other phases are associated with anorthoclase in split BH86N/33(B. Usually anorthoclase is strongly associated with other feldspars, so anorthoclase has an unusual occurrence within sample BH86N/33.

Table *ma_clast_measure* describes a lithic with a thin section area of 2.6 mm^2, assigned a *clast_ID* of *LI4* in split BH86N/33(B, as a lava of the volcanics of Stonewall Mountain. Within Appendix C are the form used to describe clasts by optical petrography as well as the completed form for split BH86N/33(B. Database table *ma_clast_alt* describes the alteration of this clast as *microgranophyric*, a type of high-temperature devitrification, as defined in table *alt_list.* In table *ma_clast_measure*, a *clast_pa_meth_code* of *B* indicates that all grain components within *LI4*, except for Fe-Ti oxides, are represented in table *ma_gr_measure*. The minerals listed within this lithic include anorthoclase, apatite, biotite, monazite, plagioclase, quartz, and sanidine; many of these minerals, the table shows, have been analyzed by electron microprobe.

Appendix C.

Forms used for detailed petrographic analysis, followed by examples for sample BH86N/33. Use of these forms requires a photomap, as shown in Figure 5. Optical analyses have been corrected for errors in original optical identifications discovered by microprobe analyses during December 1997. Areas are shown for examples as they are entered into forms, for convenience and clarity, in units of 0.0001 mm^2.

Point Count, petrographic methods, and notes for split_ID:

Meth	Mag nif	light	grid	TS area		Meth	Ma gnif	light	grid	TS area

Min ID	Meth	Total pts	Min pts	Min ppm	Ra nk		Min ID	Meth	Total pts	Min pts	Min ppm	Ra nk

ppmV = 0 method: components:

Lithology, alteration:
TS Narrative:

Clasts in split_ID:

Clast ID	Clast code	Clast area	Area meth	Geol unit	Lith	Altn	Me th	Clst cts	Anl yst	Anal date

Minerals in split_ID: page   of

Grain ID	Clst PA	Host ID	Min ID	Min area	Textur	Min Host	Min cts	Pr ver	Anl yst	Anal date

Point Count, petrographic methods, and notes for split_ID: BH86N/33(B

Meth	Mag nif	light	grid	TS area		Meth	Ma gnif	light	grid	TS area
1	500	RT	1.17576	343						

Min ID	M eth	Total pts	Min pts	Min ppm	Ra nk		Min ID	Met h	Total pts	Min pts	Min ppm	Ra nk
SD	1	292	51.04	174800	1		AP	A			327	1
AO	1	292	1.975	6765	1		BT	A			2186	1
PL	1	292	6.972	23880	1		CX	A			826	1
VP	1	292	41	140411	1		OL	A			150	1
LI	1	292	2	6849	2		SN	A			0.3	1
VO	1	292	29	99315	1		PE	A			20	1
BT	1	292	1	3425	2		PO	A			0.3	1
CX	1	292	2	6849	2		ZR	A			129	1
MT	1	292	2	6849	2		IL	E			290	1
QZ	1	292	1	3425	1		MT	E			1575	1
LI	L			8413	1		HN	L			1000	1

ppmV = 0 method: 1   components: HN,OX,OL,NA,IL,AY,SU,MM
                         A   OX,NA,SN,AL,MN,PY,MM

Lithology, alteration: MG/VP
TS Narrative: Abundance for HN from grains examined is 824 ppmV.

Clasts in split_ID: BH86N/33(B   **page   1   of   1**

Clast ID	Clast code	Clast area	Area meth	Geol unit	Lith	Altn	Me th	Clst cts	Anlyst	Anal date
LI1	LI	1008	S		LA	GS	A	1	RGW	23Aug97
LI2	LI	688	S		VOL	QC	A	0		6Sep97
LI3	LI	836	S				A	0		24Aug97
LI4	LI	25760	S	Ts	LA	MG	B	1		13Dec97
LI5	LI	565	S		GR		A	0		7Sep97

Grain ID	Clst PA	Host ID	Min ID	Min area	Textur	Min Host	Min cts	Pr ver	Anlyst	Anal date
1			SD	762			1	Y	RGW	23Aug97
1			GZ	1	M		0	N	RGW	23Aug97
2			SD	390			1	Y	RGW	23Aug97
O1		PC1	MT	67	A		1	N	RGW	23Aug97
VP1A			VK	396	M		1	Y	RGW	23Aug97
27		PC	AO	1390			0.48	Y	RGW	14Dec97
27		PC	AO	1489			0.52	Y	RGW	14Dec97
33		PC2	AO	8560			1.39	Y	RGW	22Dec97
33		PC2	SD	3720			0.61	Y	RGW	22Dec97
43			AO	1010		SD	0.19	Y	RGW	22Dec97
43			SD	4350			0.81	Y	RGW	22Dec97
57		PC	PL	805	W		0.82	Y	RGW	22Dec97
57		PC	AO	178			0.18	Y	RGW	22Dec97
VP3	A	LI4	AO	309	R		1	Y	RGW	13Dec97
A4	A	LI4	BT	80	F		0	N	RGW	25Aug97
A4	A	LI4	AP	1		BT	0	N	RGW	25Aug97
A4	A	LI4	AP	1		BT	0	N	RGW	25Aug97
B4	A	LI4	BT	68	F		0	N	RGW	25Aug97
C4	A	LI4	MN	12			0	N	RGW	13Dec97
D4	A	LI4	QZ	235			0	Y	RGW	25Aug97
E4	A	LI4	QZ	565			0	Y	RGW	25Aug97
F4	A	LI4	AO	421	R		0	Y	RGW	13Dec97
I4	A	LI4	PL	590	R		0	Y	RGW	13Dec97
G4	A	LI4	PL	347	A		0	Y	RGW	25Aug97
G4	A	LI4	SD	186	A		0	Y	RGW	25Aug97
H4	A	LI4	PL	48	A		0	Y	RGW	13Dec97
J4	A	LI4	PL	26	A		0	Y	RGW	13Dec97
K4	A	LI4	SD	11	A		0	N	RGW	25Aug97
O7			MT	25	A		0	N	RGW	24Aug97
O7			ZR	1			0	N	RGW	24Aug97
NE/26			AP	111			0	Y	RGW	2Sep97
NE/26			AP	31			0	N	RGW	2Sep97
U			CX	167		HN	0	Y	RGW	13Dec97
U			MT	45	A		0	N	RGW	2Sep97
U			ZR	13			0	Y	RGW	2Sep97
U			HN	15	E/M		0	Y	RGW	13Dec97
AL			HN	34	M		0	Y	RGW	14Dec97
AO			HN	35	M		0	Y	RGW	14Dec97

Appendix D. Examples of NTS database queries using SQL (Structured Query Language)

1. Petrographic Data

Description of Analysis

Accessory minerals other than apatite and zircon are consistently present within certain stratigraphic units and are consistently absent within others. In many instances, the presence or absence of a key accessory mineral provides the most definitive difference between two strongly associated units. The most well known example is the presence of sphene in Ammonia Tanks Tuff (Tma) in contrast to its absence in Rainier Mesa Tuff (Tmr), as described by Byers et al. (1976a). Another striking difference between these two units is the presence of monazite in Rainier Mesa Tuff in contrast to its absence in Ammonia Tanks Tuff (Warren et al., 1989b). The monazite contents of these units, determined by detailed petrographic analyses, is shown in Figure D-1 using analyses extracted from the database.

Important considerations in this comparison are stratigraphic unit, sample type, concentration units, and petrographic method. Selecting stratigraphic units Tma and Tmr and all daughters (e.g., Tmrpl) ensures proper selection of the desired unit and all subunits, but includes mafic tephras at the base of Tmr that are inappropriate for comparison (Tmrd and Tmra), which are eliminated from the comparison set below. Volume concentrations are representative only within certain sample types, such as representative cuttings (sam_type_code *DA* in database table *sample*), core (code *C*), and Hunt sidewall (*HS*), and not within others such as mineral separates from core (code *CM*). Certain petrographic analyses yield semiquantitative results expressed as the number of grains observed (units code *G* in database table *pa_measure*), and so are not included in the comparison of quantitative results below. Finally, uncertainties in quantitative analyses for accessory mineral abundances depend strongly on the method of analysis; uncertainties are narrowest for *pa_meth_code A* in database table *pa_measure*. For most comparisons similar to that shown below, selection of data should consider the method of petrographic analysis, but all analyses for monazite currently within the database have been determined via *pa_meth_code A*.
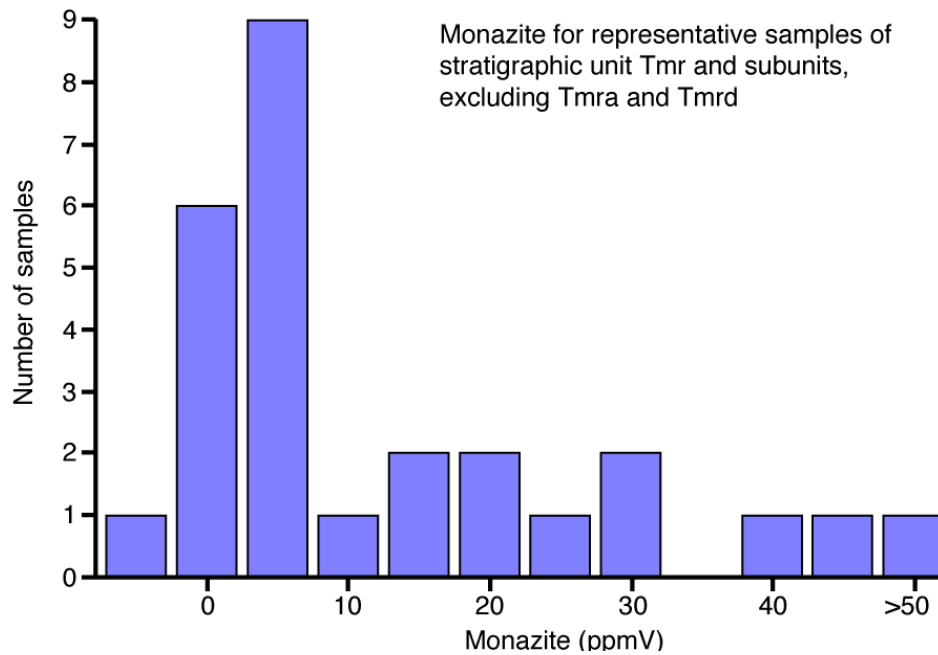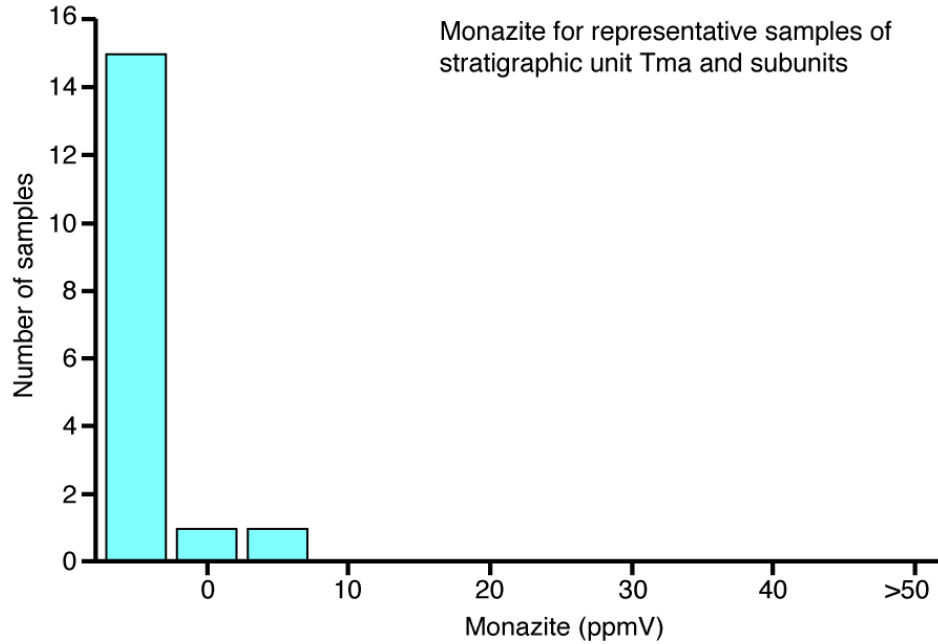
Figure D-1. Characteristic monazite abundances applied to distinguish between Ammonia Tanks Tuff (Tma) and Rainier Mesa Tuff (Tmr).

Description of Query

This query extracts petrographic abundance data for certain sample types of a given mineral within a particular stratigraphic unit. The query extracts data from three database tables: *pa_measure, pa_split*, and *sample*, which must be joined through common fields: *spl_id* and *sam_id*. A set of nested subqueries is used to identify petrographic splits for samples from the appropriate stratigraphic unit: Tma, and well

45

as any subunits. These subunits are obtained through the parent-child relationship: *strat_group_code:strat_code*. The query and query results are provided in Figure D-2.

```
A) QUERY
  SELECT pa_split.spl_id, sample.sam_id, sam_type_code, strat_code, comp_code,
    comp_value
    FROM pa_measure, pa_split, sample
    WHERE pa_measure.spl_id = pa_split.spl_id
    AND pa_split.sam_id = sample.sam_id
    AND sam_type_code IN ('C','DA','F','H','HS','O','PS','SC','T')
    AND comp_code = 'MN'
    AND pa_split.spl_id = ANY
      (SELECT spl_id
        FROM pa_split
       WHERE sam_id = ANY
          (SELECT sam_id
            FROM sample
          WHERE strat_code = ANY
            (SELECT strat_code
              FROM strat
              START WITH strat_code = 'Tma'
              CONNECT BY PRIOR strat_code = strat_group_code
            )
          )
      );
```

```
B) RESULTS

spl_id              sam_id           sam_type_code    strat_code    comp_code    comp_value
-------------       --------------   -------------    ----------    ----------   ----------

U3LA-850S(2         U3LA-850S        HS               Tmab          MN              0
UE19X-221.7(C       UE19X-221.7      C                Tmab          MN              7.7
85FB53(A            85FB53           O                Tmap          MN              0
U7BD-850S(2         U7BD-850S        HS               Tmap          MN              0
UE19X-145(B         UE19X-145        C                Tmap          MN              0
UE14A-1190D(2       UE14A-1190D      DA               Tmap          MN              0
U7BD-750S(1         U7BD-750S        HS               Tmap          MN              0
U7BD-720S(2         U7BD-720S        HS               Tmap          MN              0
85FB51(A            85FB51           O                Tmar          MN              0
85FB61-WR(C         85FB61-WR        O                Tmar          MN              0
CS10/86(A           CS10/86          O                Tmar          MN              2.6
UE19X-75(B          UE19X-75         C                Tmar          MN              0
U19Y\S-200S(2       U19Y\S-200S      HS               Tmar          MN              0
RW18B10(C           RW18B10          O                Tmar          MN              0
MRH/93BH/20A(2      MRH/93BH/20A     O                Tmar          MN              0
ER30/1-1300D(2      ER30/1-1300D     DA               Tmar          MN              0
85FB61-WR(B         85FB61-WR        O                Tmar          MN              0
```

Figure D-2. Selection of petrographic measurements using nested subqueries and parent-child relationships (hierarchical queries).

2. Mineralogic Data

Description of Analysis

Mineral compositions determined by electron microprobe generally fall within narrow ranges for each stratigraphic unit (Warren et al., 1983b; Warren et al., 1989b). One important use of such mineral compositions is to define and correlate stratigraphic units, as described in section IV. The most useful mineral for such purposes is K-spar, which occurs within most volcanic units of the SWNVF. The K-spar of volcanic units of the SWNVF is invariably sanidine, but occasionally anorthoclase also occurs. Figure

D-3 compares the combined potassium and barium contents of K-spar, expressed as mole% orthoclase (OR) plus celsian (CN) end member contents, between Tmr and Tma. Except for a single sample confidently assigned as Tmr (U19AB-600D), all samples of Tmr contain dominant sanidine within a narrow range from an OR+CN content of 62 mol%, as shown below. In comparison, all samples of Tma contain dominant sanidine with an OR+CN content centered at 47 mol%, and additionally anorthoclase with an OR+CN content centered at 22 mol%. Some K-spar compositions do not match dominant compositions owing to incorporation of xenocrysts from underlying units or to strong Na-enrichment (K-depletion) of rims by alkali diffusion during cooling, producing albitic rims as described by Warren et al. (1984). As seen in Figure D-3, albitic rims are typically observed for sanidine of Tmr, but not for Tma.

Stratigraphic units are exactly as for the query above. In contrast, sample type does not affect K-spar chemistry, and so need not be considered. The quality of the petrographic analysis is also irrelevant, so the sample set can include analyses from petrographic splits with acceptable analyses (table *pa_split*), or splits with unacceptable analyses (table *xx_pa_split*). Because Ba proxies for the dominant K, it is important to exclude analyses of K-spar lacking Ba; K-spar analyses require analysis of K (Table 9).

The acceptance criteria for microprobe analyses (Table 9) ensure accurate analyses. Analyses that do not meet these criteria can lead to erroneous conclusions. Mills (1991), using analyses from database table *xx_probe_measure* that violate these criteria, concluded that K-spars from Tma and Tmr are compositionally indistinguishable.
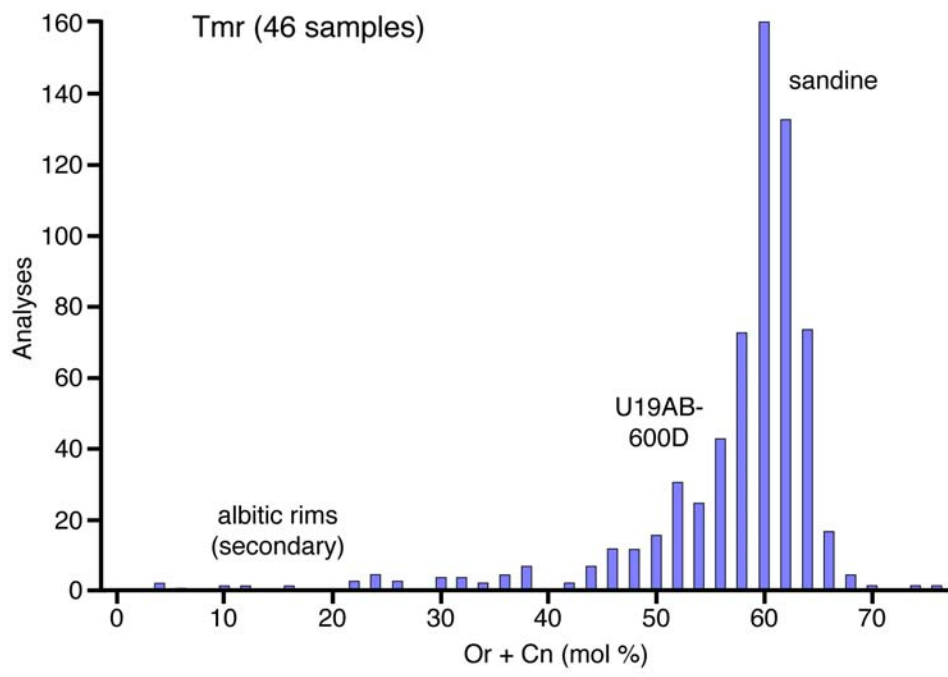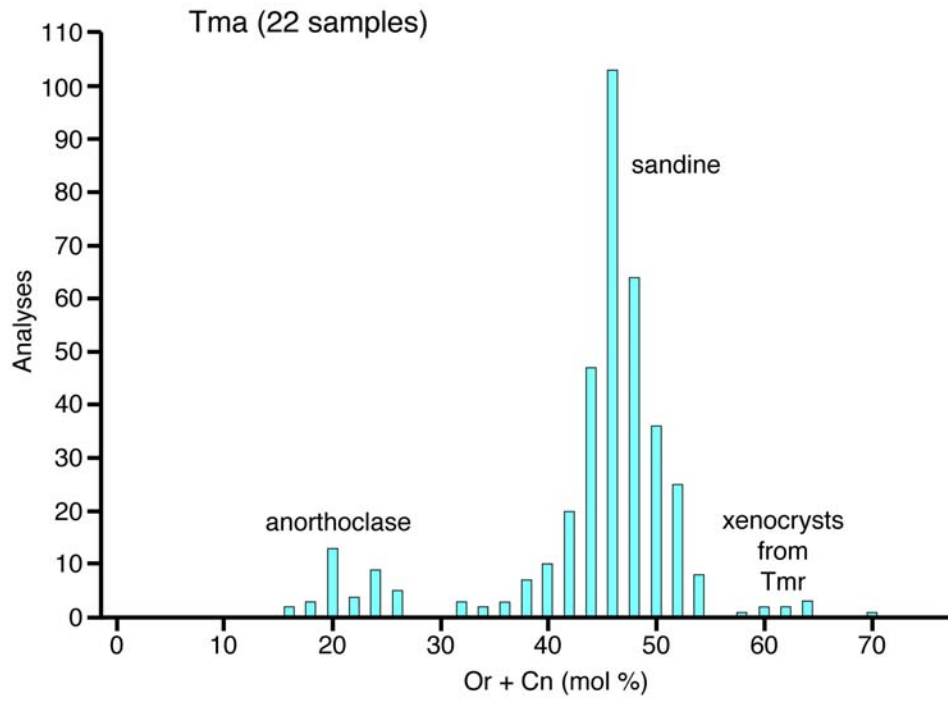
Figure D-3. Characteristic sanidine compositions (OR + CN) for the Ammonia Tanks Tuff (Tma) and Rainier Mesa Tuff (Tmr), which allow their mineralogic differentiation.

Description of Query

This query extracts measurements of combined mineral abundances for certain grain components within a particular stratigraphic unit. The query extracts data from table *probe_end_members*.   A complex subquery containing two nested sets of subqueries is necessary to identify grain components for samples from the appropriate stratigraphic unit: Tma, and well as any subunits. The two sets of subqueries extract split ids (*spl_id*) from tables: *pa_split* and *xx_pa_split* (superceded or erroneous split information) to identify the full set of grain components which may have good mineral abundance measurements. These sets of split ids are combined through a UNION and then used to identify grain components which have measurements for either SD, AO or KF.   Grain components identified by the subquery are then used to extract measurement values (*end_member_value*) from the table *probe_end_members* for end members: OR and CN. As there is a requirement that both OR and CN values be present in order for the grain component to be included in the analysis, both of these end member values are extracted from the database. These end member values are summed by GROUPing results by grain component and extracting only those grain components HAVING both end members present (COUNT = 2) . The query and query results are provided in Figure D-4.

```
A) QUERY
        SELECT gr_comp_id, rep_id, SUM (end_member_value), COUNT (*)
          FROM probe_end_members
          WHERE end_member_code IN ('OR','CN')
        AND gr_comp_id = ANY
          (
            SELECT gr_comp_id
              FROM ma_gr_measure
              WHERE gr_comp_code IN ('SD','AO','KF')
            AND spl_id = ANY
              (SELECT spl_id
                FROM pa_split
                WHERE sam_id = ANY
                  (SELECT sam_id
                    FROM sample
                    WHERE strat_code = ANY
                      (SELECT strat_code
                        FROM strat
                        START WITH strat_code = 'Tma'
                        CONNECT BY PRIOR strat_code = strat_group_code
                      )
                  )
                )
              UNION
              SELECT spl_id
                FROM xx_pa_split
                WHERE sam_id = ANY
                  (SELECT sam_id
                    FROM sample
                    WHERE strat_code = ANY
                      (SELECT strat_code
                        FROM strat
                        START WITH strat_code = 'Tma'
                        CONNECT BY PRIOR strat_code = strat_group_code
                      )
                  )
                )
            )
          )
        GROUP BY gr_comp_id, rep_id
        HAVING COUNT (*) = 2
      ;
```

```
B) RESULTS
        gr_comp_id      rep_id      SUM (end_member_value)      COUNT (*)
        ----------      ------      -------------------------   ----------
        25086             1                45.2599                  2
        25089             1                46.601                   2
        25089             2                45.2128                  2

             .
             .
        721783            1                40.38                    2
        721784            1                51.94                    2
```

Figure D-4. Selection of summed mineralogical measurements using unions, nested subqueries and
parent-child relationships (hierarchical queries).

3. Chemical Data

Description of Analysis

At Yucca Mountain, samples of mafic-poor Calico Hills Formation (Thp) that are zeolitic and have major
amounts of clinoptilolite are often strongly depleted in Na and enriched in Ca compared to samples that
are not zeolitic (Broxton et al., 1987). At Pahute Mesa, north across Timber Mountain from Yucca
Mountain, similar samples of Thp are generally only slightly depleted in Na and enriched in Ca, as seen in

Table D-1. For discussion of the correlation of Thp across Timber Mountain, see Figure 13 and discussion in text. This chemical difference measures the extent of cation exchange, Ca for Na, in clinoptilolite within the two regions.

Location	Sites	CaO		K2O		Na2O	
		avg	unc	avg	Unc	avg	Unc
Pahute Mesa	8	1.14	0.44	4.22	0.59	2.56	0.72
Yucca Mountain	55	1.79	0.14	4.83	0.36	1.12	0.13

Table D-1. Average chemical values and their uncertainties for zeolitic mafic-poor Calico Hills Formation. Values from each site are averaged to provide a single value that is averaged with values from other sites. Uncertainties are twice the standard error of the mean.

Important considerations in this comparison are stratigraphic unit, sample type, and location of the sample. The selection of stratigraphic unit, Thp, is simple. Similar to the first query, only representative sample types provide chemical values appropriate for comparison. A simple geographic demarcation divides the analyses into those from Pahute Mesa, which have UTM northings >4100000 m, versus those from Yucca Mountain, which have northings <4100000 m.

Among other possible considerations are analysis type, a more detailed consideration of sample type, and treatment of analyses below detection limits. Almost all analyses for this comparison were obtained by X-ray fluorescence (XRF) or by neutron activation analysis (NAA). For the elements compared, uncertainties that accompany most of the analyses summarized below in database table *ca_measure* indicate that XRF analyses are generally superior. The samples within each geographic set include outcrop and subsurface, which might have a significant chemical effect. Although no analyses for the three elements below are below detection limits, many analyses for MgO fall below detection limits, so averages for MgO must consider such values. Because detection limits for NAA analyses of MgO are very poor, such analyses are probably best ignored, but XRF analyses are very sensitive for MgO, and values below detection limits certainly must be treated. Values below detection limits can be included to provide reasonably accurate averages when relatively small fraction of the analyses (certainly <25%) fall below such limits; a value of half the detection limit is typically assumed for analyses below such limits. To evaluate differences for MgO between Pahute Mesa and Yucca Mountain clearly requires familiarity with chemical analyses. This example illustrates the following caveat: *it is very important for the user of this database to be familiar with analytical methods for each type of data used, and with the types of samples valid for the planned application.*

Description of Query

This query extracts measurements of average chemical abundances for certain for geographic locations within a particular stratigraphic unit. The query extracts data from tables: *ca_measure*, and *location*, using table *loc_sam_split* to relate measurements to locations. A nested subquery identifies chemical splits from the appropriate stratigraphic unit: Thp. The ca_measure table contains NULL value entries for *oxide_value* measurements that failed to identify the presence of a chemical. For this case, a quantity equal to one half of the Lower Detection Limit (*oxide_ldl)* for the particular analysis and/or measurement technique is used to quantify the chemical abundance. In order to extract abundances for all measurements including NULLs, and then assign an average value at a geographic site, a set of temporary views is created. The first two views (*temp1, temp2*) extract non-NULL and NULL measurements, respectively. View *temp3* combines the results of *temp1* and *temp2* for the final select statement in which

the measurements are grouped by location and averaged. The query and query results are provided in Figure D-5.

```
A) QUERY
        CREATE VIEW temp1 ( loc_id, utm_e, utm_n, oxide_value )
          AS SELECT location.loc_id, utm_e, utm_n, oxide_value
          FROM ca_measure, loc_sam_split, location
          WHERE ca_measure.spl_id = loc_sam_split.spl_id
          AND loc_sam_split.loc_id = location.loc_id
          AND ca_measure.oxide_code = 'MgO'
          AND ca_measure.oxide_value IS NOT NULL
          AND ca_measure.spl_id = ANY
            (SELECT spl_id
               FROM loc_sam_split
               WHERE sam_id = ANY
                 (SELECT sample.sam_id
                    FROM sample, sample_alt
                    WHERE sample.sam_id = sample_alt.sam_id
                    AND strat_code = 'Thp'
                    AND sam_type_code IN
                       ('C','DA','F','H','HS','O','PS','SC','T')
                    AND alt_code = 'ZC'
                    AND alt_rank IN (1,2)
                 )
            );

        CREATE VIEW temp2 ( loc_id, utm_e, utm_n, oxide_value )
          AS SELECT location.loc_id, utm_e, utm_n, oxide_ldl / 2
          FROM ca_measure, loc_sam_split, location
          WHERE ca_measure.spl_id = loc_sam_split.spl_id
          AND loc_sam_split.loc_id = location.loc_id
          AND ca_measure.oxide_code = 'MgO'
          AND ca_measure.oxide_value IS NULL
          AND ca_measure.spl_id = ANY
            (SELECT spl_id
               FROM loc_sam_split
               WHERE sam_id = ANY
                 (SELECT sample.sam_id
                    FROM sample, sample_alt
                    WHERE sample.sam_id = sample_alt.sam_id
                    AND strat_code = 'Thp'
                    AND sam_type_code IN
                       ('C','DA','F','H','HS','O','PS','SC','T')
                    AND alt_code = 'ZC'
                    AND alt_rank IN (1,2)
                 )
            );

        CREATE VIEW temp3 ( loc_id, utm_e, utm_n, oxide_value )
         AS
           SELECT loc_id, utm_e, utm_n, oxide_value
              FROM temp1
           UNION
           SELECT loc_id, utm_e, utm_n, oxide_value
              FROM temp2;

        SELECT loc_id, utm_e, utm_n, AVG ( oxide_value )
           FROM temp3
         GROUP BY loc_id, utm_e, utm_n;
```

```
B) RESULTS
   loc_id          utm_e       utm_n      AVG (oxide_value)
 --------       --------     --------    -----------------
   3/15/82/2      545202.3    4084927.99     .14
   3/15/82/4      545230.38   4084888.37     .19
   3/15/82/6      545271.9    4084878.43     .28
   3/15/82/7      545290.49   4084833.67     .24
   3/15/82/8      545290.49   4084833.67     .28
   3/15/82/9      545342.29   4084932.54     .2283
   4/16/85/3      552196.51   4085307.46     .3029
   CRCH/10/SNL    557317.61   4081512.06     .415
   CRCH/8/SNL     557373.97   4081512.25     .19
      .
      .
      .
   UE20E1         548110.44   4129980.72     .346
   UE20F          545400.82   4124900.35     .08
   UE25A1         549934.73   4078317.2      .2125
   USWG1          548298.71   4080017.97     .3231875
   USWG2          548138.56   4082553.83     .07
   USWG4          548937.85   4078590.12          .045
```

Figure D-5. Selection of averaged chemical measurements for geographic sites using views with unions and nested subqueries.

Table 9. Acceptance criteria for microprobe analyses within this database. Criteria have been developed during 20 years by Rick Warren, based on published analyses (Deer et al., 1962a-c; Papike, 1987, 1988) and practical limits for microprobe analysis. Criteria have not been applied rigorously, but >99% of the acceptable analyses within this database conform. Acceptable analyses must include essential elements, with a few exceptions denoted by asterisks allowed within the database. Monitor elements are undetectable by microprobe analysis, but usually associated with alteration or with secondary fluorescence of adjacent minerals; analyses for such elements above the indicated values indicates a problem and the analysis should be considered unacceptable. Values shown for monitor elements apply to oxide concentrations; asterisks denote elements that are poor monitors, but if analyzed, should provide the value shown. The molecular basis for structural criteria is 24 oxygens, except for hornblende, based on 23, and biotite, based on 22. Tetrahedral cations (t) are Si, Al, P, Nb, and Ti in glass only, and octahedral cations (o) are all all other cations. The charge ratio R is the ratio of charge deficiency within the tetrahedral site to the total charge of cations within the octahedral site. The charge deficiency within the tetrahedral site is the sum of trivalent cations minus the sum of pentavalent cations. Concentrations of FeII and FeIII in magnetite and ilmenite are calculated from Spencer and Lindsley (1981); values are allowed to deviate from their structural basis, shown below, only when all Fe occurs as FeII. The structural criterion for glass is based on Warren (1983a).

Mineral	elements analyzed as oxides			Acceptable Totals (%)	Structural Criteria
	essential	recommend	monitor		
feldspar	Na,Al,Si,K,Ca,FeIII*,Ba*	Sr	Mn*,Ni*,Cr* < 0.1% Ti* < 0.3%	97.5-102	o 2.85-3.15 (except adularia) R 0.95-1.05
biotite	Na,Mg,Al,Si,K,Ti,FeII,Ba*	F,Cl,Mn	Ca < 0.2%	92-102.5	o 6.5-8.5, t 7.5-8.7 K2O+0.614 X BaO > 7%
hornblende	Na*,Mg,Al,Si,K,Ca,Ti,FeII	F,Cl,Mn		94-102	CaO 9.5-13.5%
clinopyroxene	Na,Mg,Al,Si,Ca,Ti,Mn*,FeII	Cr	K* < 0.1%, Ba* < 0.3%	97-102.5	o < 8.4 t > 7.9
orthopyroxene	Mg,Al,Si,Ca,Ti,Mn*,FeII	Na,Cr	K* < 0.1%, Ba* < 0.3%	97.5-103	o < 8.3 t > 7.85
olivine	Mg,Si,Ca,Mn*,FeII	Ni,Zn	Na*,Al,P*,K* < 0.1% Ti < 0.2%, Ba* < 0.3%	98-104	o 11.6-12.4 t 5.8-6.2
ilmenite	Mg,Al,Ti,Mn*,FeII,FeIII	Cr,Zn,Nb	Si,Ca < 0.2%, Zr < 0.3%	96-103	o 6, t 12
magnetite	Mg,Al,Ti,Mn*,FeII,FeIII	V,Cr,Zn	Si,Ca < 0.2%, Zr < 0.3%	96-103	o 8, t 8
glass	Na,Mg*,Al,Si,K,Ca,Ti*,FeIII	F,P,Cl,Mn,Ba		<102	R >0.95
zeolite	Na,Mg*,Al,Si,K,Ca	FeIII,Ba	Mn* < 0.1%, Ti* < 0.2%	<102	R 0.85-1.05
silica	Na,Al,Si,K*,Ca,FeIII		Cr*,Mn*,Ni* < 0.1%, Ti < 0.2%	97-102.5 (except OP <99)	