Chapter 4 Hydrographic Data Formats

4.1 Data Files

Each expedition participating in the WOCE hydrographic programme should produce three to five data files documenting the water sampling. Additional files containing the underway data sampling are also needed, and these are described in Chapter 5. These files are requested from the **chief scientist** six months after the end of each cruise:

Final Cruise Report

The *first* file is the cruise report text (—.DOC) documenting the events of the cruise, including an expanded and completed version of the previously submitted chief scientist's report, station inventory, a description of problems encountered during the cruise, and sections from *all* the various investigators describing their techniques and instrumentation, constants used, calibration and blank data, and pertinent references including the underway data. Chief scientist's reports are described in Section 3.2.2 on page 27 and an outline for the —.DOC file is given in Table 3.4. A sample —.DOC file is provided as Appendix C. A standard reporting protocol for measurements is given in Appendix D. Thorough and consistent documentation is considered an essential part of every WOCE cruise and it is requested that the outline in Table 3.4 on page 28 be followed.

It is suggested that much of the —.DOC file information be assembled during the cruise.

Station Positions

The *second* data file is an updated and corrected station summary (—.SUM) file as described in Section 3.3 on page 29. An example of a —.SUM file is given in Table 3.5. All station location and time information is contained in the —.SUM file.

This file should be assembled as the cruise progresses.

Bottle Data

Normally, the *third* data file (—.SEA) contains the results from *all* the small volume water sample measurements made during the cruise. The format for the water sample data is described in Section 4.3. Columns, and a quality flag, for every WOCE parameter measured on the cruise should be included in the —.SEA file even though some of the data may be delayed (quality flag = 1). Parameters other than the WOCE ones may be included in the —.SEA file at the option of the chief scientist. That option is recommended if the WOCE parameters, for example, salinity and temperature, are necessary to evaluate the supplemental measurements so as to provide all the available data in a single file.

Quality flags are optional for non-WOCE parameters.

A template for the —.SEA file should made *before* the cruise and the data added as the cruise progresses. The WHPO can provide such a template after receipt of a cruise plan.

All participating PIs should be given a copy of the preliminary —.SEA file at the end of the cruise.

CTD Data

The *fourth* set of data files, described in Section 4.4, contains the CTD data from the cruise as well as a quality word for each record showing the investigator's evaluation of their data quality. It is expected that CTD data will be reported in a uniform pressure series in order of *increasing* pressure with a pressure resolution of 2 dbar. Quality flags are required for all WOCE CTD parameters, but are optional for others.

Due to the volume of the CTD data, it is a fairly common practice to record the CTD data from a single station on a single file. If the CTD data are sent to the WHPO on tape it may be possible to fit[1] all the individual CTD data files from a cruise on a single tape or, alternatively, floppy disks containing the CTD data for a small number of stations may be submitted. Data may also be sent to the WHPO via ftp (see Appendix A).

CTD data are also subjected to the DQE process.

Software programs are necessary to format CTD data. Please contact the WHPO for help if you don’t have them.

Data from Large Volume Water Bottles

If large volume sampling is done on the cruise then a *fifth* data file is expected from the chief scientist, or designated individual, containing the data from the large volume water samples. The format for the large volume water sample data is described in Section 4.3.1 on page 42.

As with the —.SEA file, a template should be made *before* the cruise and data added as the cruise progresses. An inventory of samples is necessary in the —.LVS file as well.

Underway Data

Additional files for any underway data should also be submitted following the guidelines given in Chapter 5.

Data Quality

Investigators are expected to evaluate the quality of their measurements and record their assessment in a quality flag as part of the data record (see Section 4.5). The data are later independently evaluated by data quality evaluators (DQEs), who assign a second quality flag to the record for each measurement. The DQE quality flags are made available to the PIs involved with the data, but are not released with the final data set. A summary of the DQE findings are published with the data report.

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1. Data compression and transmission programs the WHPO can decode are listed in Appendix E.

4.2 Water Sample Identification

If a uniform, global hydrographic data set is to be compiled during WOCE it is axiomatic that the time and physical location where every sample in the data set was taken be accurately known and uniquely identified. In order to accomplish this we have evolved the following scheme:

First, each cruise in the data set is given a unique identifier, the EXPOCODE defined in Section 3.3 on page 29. The EXPOCODE must appear in every file [—.DOC (Section 3.2 on page 27), —.SUM (Section 3.3 on page 29), —.SEA and —.LVS (Section 4.3 on page 38), —.CTD (Section 4.4 on page 49), and etc.] submitted to the WHPO or other WOCE Data Assembly Center (DAC).

Secondly, each station on a cruise must be given a unique (alphanumeric) identifier. Repeat and time series cruises often use the same station number (STNNBR) on sequential cruises and that presents no difficulties as long as each cruise is given a unique EXPOCODE. In order to gauge the accuracy of the station position we ask that position, time, and the uncorrected depth be given in the—.SUM file for the beginning, bottom, and end of every hydrographic cast. That allows an estimate of the drift of the ship and whether or not the ship drifted across significant topography during the station. When unique coordinates are required for the station position the bottom time is normally used.

The *third* identifier in the string is a cast number (CASTNO). For the sake of uniformity we ask that at each station on each cruise the cast numbers begin with 1, and each over the side operation be given a separate cast number. If a station is reoccupied later during the same cruise, and the same station number is used, the cast numbers should increment upward from the last cast number at the same station. In no case should the —.SUM file contain the same STNNBR and CASTNO on the same cruise. STNNBR and CASTNO appear in all —.SUM, —.SEA, —.CTD, and —.LVS files submitted to the WHPO and must be used consistently in each file in which they appear. For purposes of the WHP database the —.SUM file is used as the key and the other files are tied to that key by EXPOCODE, STNNBR, and CASTNO.

The *fourth* identifier in the string is the sample number (SAMPNO). Many groups use the sample number to identify the rosette position of the bottle from which water samples are drawn while on deck. Other groups are using schemes where unique and consecutive sample numbers are printed on sticky labels before the cruise. For each bottle sampled, an identifying number is assigned and identical multiple labels are printed beforehand to allow this same number to be attached to each and every subsample drawn from the bottle and, thus, track the sample collection bottles as well. Other schemes are possible and useful. Whatever scheme is used it is critical that the same numbering scheme be used by all participants on the cruise. Great confusion arises if one group uses one sample numbering scheme and another group uses a different one on the same cruise (as has happened). Water samples are analyzed at various times and places, sometimes years after the cruise, as is the case with AMS ^{14}C and helium/tritium samples, for example. Inconsistent identification of the bottle from which the sample was drawn can make it difficult, if not impossible, to merge the various measurements into the database when the data are finally assembled either by the chief scientist or the WHPO.

In summary, each bottle sampled should be identified by a combination of EXPOCODE, STNNBR, CASTNO, and SAMPNO. This combination must be capable of uniquely identifying every water sample collected throughout WOCE. Also, for uniqueness, these identifiers must be composed only of numbers and UPPERCASE letters and cannot contain any embedded blanks.

For —.SEA and —.LVS files the bottle number (BTLNBR) is also required in order to uniquely identify the particular device used to collect the water sample. The bottle number is defined as: (1) the permanent, unique serial number (alphanumeric) stamped or engraved on the barrel of the bottle from which the water samples are drawn or, alternatively, (2) as a unique alphanumeric identifier assigned to only that device over the duration of the expedition. A unique serial number can be useful because it allows a group to track repairs and parts replacement for individual bottles. Note that for every water sample, the BTLNBR has an associated quality flag in the WHP data format to indicate problems associated with the sampling device that were noted either at the time the samples were drawn, or found during later analysis. The combination of BTLNBR and its quality flag allows 'problem' bottles to be identified and tracked. For example, individual bottles may leak chronically, may contaminate the samples being taken, e.g., chlorofluorocarbons, or may consistently mistrip or otherwise malfunction. Such bottles are usually discovered early in a cruise and replaced on the rosette for that cruise. However, the defective bottles may subsequently be reused on following legs with different personnel, but using the same equipment, if a replacement bottle is needed. Hence, users are urged to maintain a tracking capability transferable to other cruises. If no manufacturer’s serial number is available for the sampling device, identifying numbers may be stamped on the bottle.

4.3 Water Sample Data Format (—.SEA and —.LVS)

In order to assemble a uniform global data set it is essential that all data be reported in consistent units to uniform standards with records containing the same information and following the same naming conventions. In order to approach that goal it is requested that standard formats be used.

The following formats are the end result of considerable debate within and external to the WHPO and the WHP Planning Committee. They are unlikely to satisfy everyone, but should provide the WHPO and, hence, the WOCE Hydrographic Programme with reasonably consistent data sets from a diverse community. The —.SEA and —.LVS files defined here are basically a list, or matrix, of all parameters measured from the water bottles and indexed by the quality flags, which define what is measured from each bottle and how well it was done.

It is the responsibility of the **chief scientist** for each cruise to *assemble* and *submit* all of the data from a WHP cruise as only they know what measurements were made and where they were made. Most WHP data should be sent to the WHPO (see Table 1.1 on page 4). The WHPO will gladly provide any advice or assistance within our power to help in cruise documentation and data assembly.

The WOCE water sample data format is not intended to be storage efficient, but, rather, to be portable and self-documenting. Cruise and position information for each cast are given in the —.SUM file and are cross-referenced with the —.SEA and —.LVS files by station number (STNNBR) and cast number (CASTNO). One water sample record is required for each bottle on each cast. Table 4.1 shows the format for each individual small volume water sample record. A column for *every* parameter (and error estimate if applicable) measured on the cruise must be included in the —.SEA (or —.LVS) file. The process seems to work best if a template with all of the requisite columns included is prepared prior to the cruise and as much data as possible from each station is added to the file during the cruise.

TABLE 4.1: WHP small volume water sample record format description

Column Headings		Units			Reporting Precision	
Parameter Number*	**Parameter Mnemonic**	**Mnemonic**	**Scientific**	**Parameter or see note no.**	**Range**	**FORTRAN Format**
	STNNBR		character	(Note 1)		A8
	CASTNO		integer	(Note 2)		5X,I3
	SAMPNO		character	(Note 3)		1X,A7
	BTLNBR		character	(Note 4)		1X,A7
	CTDRAW	DBAR	decibar	(Note 5)	0,11000	1X,I7
	CTDPRS	DBAR	decibar	Pressure	0,11000	F8.1
	CTDTMP	ITS-90[3]	°C (ITS_{90})	Temperature[3]	–2,35	F8.4
	CTDSAL[1†]	PSS-78[5]	PSS-78	Salinity[1]	0,42	F8.4
	CTDOXY[†]	UMOL/KG	µmol/kg	Oxygen	0,500	F8.1
	THETA	DEG C[3]	°C (ITS_{90})	(Note 6)	–2,35	F8.4
1	***SALNTY***[1]	PSS-78[5]	PSS-78	Salinity[1]	0,42	F8.4
2	***OXYGEN***	UMOL/KG	µmol/kg	Oxygen	0,500	F8.1
3	***SILCAT***	UMOL/KG	µmol/kg	Silicate	0,250	F8.2
4	***NITRAT***[8]	UMOL/KG	µmol/kg	Nitrate[8]	–0.1,47	F8.2
5	***NITRIT***[8]	UMOL/KG	µmol/kg	Nitrite[8]	–0.1,15	F8.2
6	***PHSPHT***	UMOL/KG	µmol/kg	Phosphate	0,5	F8.2
7	***CFC-11***[5]	PMOL/KG	pmol/kg	Freon-11™	–0.1,15	F8.3
8	***CFC-12***[5]	PMOL/KG	pmol/kg	Freon-12™	–0.1,15	F8.3
27	***CFC113***	PMOL/KG	pmol/kg	Freon-113™	–0.1,1.5	F8.3
28	***CCL4***	PMOL/KG	pmol/kg	Carbon tetrachloride	–0.1,20	F8.3
	REVPRS	DBAR	decibar	(Note 7)	0,11000	F8.1
	REVTMP[3]	ITS-90	°C (ITS_{90})	(Note 8)	–2,35	F8.3
9	***TRITUM***[2]	TU	TU[7]	Tritium[2]	–1,100	F8.3
10	***HELIUM***	NMOL/KG	nmol/kg	Helium[2]	1,3	F8.4
11	***DELHE3***[2]	PERCNT	%	Helium[2]	–10,100	F8.2
12	***DELC14***[2]	/MILLE	0/00	^{14}Carbon [2]	–300,250	F8.1
13	***DELC13***[2]	/MILLE	0/00	^{13}Carbon [2]	–5,5	F8.1
15	***ARGON***	UMOL/KG	µmol/kg	Argon	5,25	F8.2
17	***NEON***[2]	NMOL/KG	nmol/kg	Neon[2]	0,10	F8.3
20	***O18/O16***[2]	/MILLE	per mille	$^{18}O/^{16}O$ ratio[2]	–5,5	F8.2
n+1[4]	↓	Additional parameters may be added as needed. If a parameter number and mnemonic are not given in Appendix G please contact the WHPO for the appropriate number in order to avoid possible conflict with other investigators.				
n+x	↓					
	Parameters requiring conversion factors or expected error data column					
9	TRITER[2]	TU	TU[7]	Tritium[2]		F8.3
10	HELIER[2]	NMOL/KG	nmol/kg	Helium[2]		F8.4
11	DELHER[2]	PERCNT	%	Helium[2]		F8.2
12	C14ERR[2]	/MILLE	0/00	^{14}Carbon[2]		F8.1
13	C13ERR[2]	/MILLE	0/00	^{13}Carbon[2]		F8.1
17	NEONER[2]	NMOL/KG	nmol/kg	Neon[2]		F8.3
	Quality Words					
	QUALT1		none	(Note 9)		*m*I1 + 1
	QUALT2		none	(Note 10)		*m*I1 + 1

Include a column for every parameter measured (or sampled for) on the cruise, including an error column if applicable. Omit those parameters not measured on your cruise. One record is required for each water bottle sampled on each cast. The individual water sample records are then compiled into a —.SEA file for submittal to the WHPO. All WOCE parameters printed in ***BOLD*** require a quality flag in the quality word. ***BTLNBR***, ***CTDSAL***, and ***CTDOXY*** also require quality flags in the quality word but the definitions for these quality words differs from the water sample flags. Quality flags are optional for non-WOCE parameters. The first data record in the —.SEA file is preceded by four header records defined in the formatting notes.

TABLE 4.1: WHP small volume water sample record format description

Footnotes

* The parameter number defined here and in Appendix G is used in the station summary (—.SUM file, Table 3.5) to identify the measurements made at this station. If no parameter number is defined in Appendix G for a measurement you wish to include please consult with the WHPO.

† CTD salinity and oxygen require quality flags whose definitions are given in Table 4.10.

1 Temperature on $IPTS_{68}$ scale must be used for calculating CTD Practical Salinity Scale (PSS-78) until a new algorithm is developed.

2 This parameter usually requires shore-based analysis that may take up to 18 months or longer.

3 Temperature should always be reported using ITS_{90} temperature scale. If, however, the ITS_{90} scale has not yet been adopted at your institution then it is permissible to report temperature using the $IPTS_{68}$ scale and the WHPO will convert your data to the ITS_{90} scale. If $IPTS_{68}$ scale is used, change the mnemonic in the header record to IPTS-68 rather than the default ITS-90.

4 Additional variables may be added. Units, precision, reproducibility (or accuracy if known), range, and format must be included in the —.DOC file.

5 This mnemonic includes a hyphen (-). Some PIs report machine-dependent problems with the use of hyphens. The WHPO will accept the data with or without a hyphen.

7 TU = Tritium units. 10^{18} times ratio of tritium atoms to hydrogen atoms.

8 Many investigators report the sum of nitrite plus nitrate. While it is preferred that they be reported separately, the sum is acceptable if clearly labeled as such by the mnemonic NO2+NO3. The required precision for the sum is 0.2% and the reproducibility is 1%. Range is –0.1 to 47 and units are µmol/kg and the format is F8.2.

Notes on Table 4.1

1. A sequential station number (alphanumeric). Station numbers *must* be unique for a cruise but may repeat on subsequent cruises along the same section or to the same station for time series.

2. The cast number: 1 = 1st cast; 2 = 2nd cast on a single station. Every over-the-side operation on a station is given a separate cast number. Cast numbers should start at 1 the first time a station is occupied on a cruise but are not reset if the same station is visited more than once on the same cruise.

3. The sample number assigned to all water samples drawn from a bottle (alphanumeric). Sample numbers may be unique for a cruise or reflect the position of the bottle on the rosette from which the samples were taken. Sample numbers are usually sequential on a cast from the deepest bottle to the shallowest bottle. In any case *all* groups *must* use the same sample numbering conventions.

4. The permanent, unique serial number of the bottle (alphanumeric) from which the water samples are drawn. Unless a bottle is changed on the rosette these numbers usually repeat from cast to cast and station to station.

5. *Optional*: The nominal CTD digital pressure *in decibars* recorded at each bottle closure. When transformed by the pressure calibrations this number would yield the CTD pressure (CTDPRS) if no mistrip occurred. However, CTDRAW is invariant regardless of calibration updates.

6. The potential temperature at the time each bottle is tripped. At present it is necessary to calculate initially as theta ($IPTS_{68}$) then convert to theta (ITS_{90}).

7. Pressure as measured by reversing thermometers if used.

8. The temperature measured by reversing thermometers if used.

9. The quality word (the string of quality flags is referred to as a quality word) identifies the quality of the measurements as defined by the investigators. All mnemonics printed in bold and assigned a parameter number require one quality flag in the quality word for a total of *m* flags, or bytes. The analyst's quality word (QUALT1) always appears as the last variable on the record in the —.SEA file as sent to the WHPO. Note that the bottle number (***BTLNBR***) also has its own independent quality flag defined in Section 4.5.1 on page 52, Table 4.8 and the bottle quality flag is always the first byte of the quality word. Also, definitions for quality flags for CTD (Table 4.10) and water sample (Table 4.9) data differ.

10. The quality word used to define the quality assurance suggested by the DQE. The DQE quality word (QUALT2) is the last variable in the final data set and is added by the WHPO after submittal of the —.SEA file. The DQE quality assurance is independent of the chief scientist or cruise participant. QUALT2 is only used internally and is dropped from the data reports and the data sent to the WHP-SAC.

For each of the groups whose data were not incorporated during the cruise, it is suggested that after the cruise the chief scientist provide a template with all of the requisite columns and available data included, and padded with –9s where data are missing and the quality flags set to 1 (sample taken) or 9 (sample not taken from this bottle) initially. These groups are then to fill in appropriate columns with their data and update the quality flags. The individual water sample records for all the groups on the cruise are then compiled into a single (—.SEA) file for submittal to the WHPO.

JGOFS parameters associated with the measurement of carbon dioxide, or other variables, in sea water may optionally be included in the —.SEA file. The standards for CO_2 measurements are presented in Table 4.2. Additional parameters are defined in Appendix G. Quality flags are optional with these parameters but their use is recommended. The definitions given in Table 4.9 should be used if quality flags are included.

TABLE 4.2: JGOFS carbon dioxide record format description for —.SEA file

Column Headings		Units			Reporting Precision	
Parameter Number*	Parameter Mnemonic	Mnemonic	Scientific	Parameter or see note no.	Range	FORTRAN Format
23	TCARBN[1]	UMOL/KG	µmol/kg	Total Carbon C_T	1100,2600	F8.1
24	ALKALI[2]	UMOL/KG	µmol/kg[3]	Total alkalinity A_T	100,2800	F8.1
25	PCO2[4]	UATM	µatm[5]	Partial pressure of carbon dioxide[4]	50,2000	F8.1
	PCO2TMP	DEG C	°C (ITS_{90})	$P(CO_2)$ equilibration temperature[4]		F8.2
26	PH		none[6]	pH: $-\log_{10}\{[H^+]/(mol/kg)\}$	7.6,8.3	F8.4
	PHTEMP	DEG C	°C (ITS_{90})	Measurement temperature for pH[6]		F8.2

Notes

* The parameter number defined here and in Appendix G is used in the station summary (—.SUM file, Table 3.5) to identify the measurements made at this station. If no parameter number is defined in Appendix G for a measurement you wish to include please consult with the WHPO.

1. Total carbon, total CO_2, and dissolved inorganic carbon (DIC) are equivalent. Current precision is 1.5 µmol/kg.

2. Current precision is 2.5 µmol/kg.

3. Units of µmol/kg of sea water are equivalent to the now obsolete microequivalents per kilogram of sea water.

4. Partial pressure of carbon dioxide in air that is in equilibrium with a sample of sea water. $P(CO_2)$ is calculated as the product of two measured terms: mole fraction of carbon dioxide in air and the total pressure at the time of equilibration. An additional complication is whether or not the mole fraction used in this calculation refers to dry or to wet air. Usage here implies wet air. It is also essential to report the temperature of equilibration. In revision 1 of this manual this parameter was reported as fugacity, fCO_2, and is changed here at the request of the JGOFS community. Current precision is 1 µatm at ~350 µatm.

5. 1 µatm = 0.101325 Pascal (N/m^2)

6. pH is a dimensionless quantity. The pH scale preferred for oceanic measurements refers to moles of total hydrogen ion per kilogram of sea water at a specified temperature. Thus, the temperature at which the measurement is made must also be reported. Current precision is 0.0010.

The data format for the —.SEA file is summarized in Table 4.3 and an example is given in Table 4.5.

Additional small volume water measurements not included in Table 4.1 may be included as long as the range, precision, and reproducibility (or accuracy if known) for those parameters is given in the —.DOC file. A standard reporting protocol is given in Appendix D. If a parameter number, with standard mnemonic and units, for the property you are measuring has not been included in Appendix G please contact the WHPO for the appropriate information in order to avoid overlap between the various investigators.

If unit conversions are required, please consult the appropriate section of the WHP Operations and Methods manual, WHPO 91-1, for the method to be used.

Some tracers require an explicit error definition, and these columns follow the parameters defined in Table 4.1 or Table 4.4.

Chief scientists may want to include a record in the —.SEA file with CTD pressure, temperature, and salinity at the level where a bottle failed to close, even though no bottle data are available, for the sake of continuity in the cast.

4.3.1 Large Volume Sampling

Parameters that require large volumes of water to measure are included in a —.LVS file that has the same format as the —.SEA file. The format is summarized in Table 4.4. Salinity and oxygen samples taken as a check from piggyback small volume bottles during large volume sampling should be reported in the —.LVS file as well.

At the option of the chief scientist, data from large volume water samples can be sent directly to the WHPO. In such cases the PI can either send a copy of the data directly to the chief scientist or ask the WHPO to forward a copy after checking the data.

4.3.2 Bottle Data Quality Evaluation

In order to monitor and define data quality in a machine-readable fashion, all parameters printed in ***BOLD*** in Table 4.1 or Table 4.4, or Appendix G, are assigned a quality flag, or byte. Quality flags are also used to provide an inventory of samples taken. Individual investigators are expected to assign the appropriate quality flag to each measurement they make. Individual quality flags, or bytes, are then assembled in the proper sequence into a quality word (QUALT1) by the *chief scientist* or their designated representatives (commonly the CTD group) aboard ship.

The bottle number (***BTLNBR***) has its own unique quality flag defined in Section 4.5.1, Table 4.8, and that quality flag is the *first* byte of the quality word attached to each water sample record.

The *second* and *third* flags of the quality word are associated with the CTD salinity (***CTDSAL***) and CTD oxygen (***CTDOXY***) values carried in the water sample files (—.SEA) if they were measured. The definitions for these quality flags are given in Table 4.10 in Section 4.5.3.

The remaining quality flags are associated with the water sample parameters and are defined in Table 4.9 in Section 4.5.2. For the —.SEA and the —.LVS files, the QUALT1 word terminates each data record. Note that if water is drawn for any measurement from a water bottle, the quality flag for that parameter must be set equal 1 initially to ensure that all water

TABLE 4.3: —.SEA and —.LVS file formatting

It is the responsibility of the chief scientist to see that all data files and cruise documentation are assembled and submitted to the WHPO.

The water sample records described in Table 4.1 and Table 4.4 are preceded by four header records:

All header and data records in the water sample file have the same length in order to facilitate reading and writing with fixed block format. The files are intended to be FORTRAN readable and only ASCII characters admissible in FORTRAN-77 should be used in the file. If preparing the file using a spreadsheet or word processing program on a personal computer, a monospaced font should be used to ensure column alignment. Upper case, or capital letters should be used exclusively to prevent possible difficulties with case-sensitive programs. For example, the degree symbol for temperature should not be used in the data files or the header records and U should be substituted for µ (as in UMOL/KG rather than µmol/kg).

- The **firs**t header record is used to tie the —.SEA and —.LVS files with the —.SUM file for the cruise. It is assumed, but not required, that a separate —.SEA or —.LVS file will be prepared for each leg of a multiple leg expedition. As illustrated in Table 4.5, the first record contains the country-ship code combined with the expedition designation mnemonic or cruise number and leg (EXPOCODE) defined in Section 3.3 on page 29. The WOCE section identification (WHP-ID) is also included together with the cruise dates. If more than one WOCE section or line is occupied during a single leg all section or line numbers should be included with the WHP-ID, for example, S01, S02, S04. The cruise dates (MMDDYY) should also be listed as illustrated in Table 4.5. Additional alphanumeric information may be included so long as the fixed record length is not exceeded. The record is then blank padded to the end-of-record (EOR). In the example in Table 4.5 an optional asterisk (*) has been used as an EOR mark.

- The **second** header record is composed of column headings defined by the unique mnemonics in Table 4.1 (—.SEA files), Table 4.4 (—.LVS files), or Appendix G, for each variable and parameter measured during the cruise, including parameters sampled during the cruise for later shore-based analysis. Omit those parameters listed in Table 4.1 or Table 4.4 that are not measured (or sampled) on the cruise. Each mnemonic is right justified in an eight (8) character field. Pad the field with leading blanks to round up to 8 characters for each variable or parameter except for the quality word (QUALT1). QUALT1 is right justified so that it defines the end-of-record (EOR), that is, the 1 in QUALT1 must be aligned above the last quality flag in the data records. This ensures that the header records and the data records have the same length. If parameters are included that are not defined in Appendix G a unique parameter number and mnemonic should be obtained from the WHPO in order to avoid overlap with other investigators.

- The **third** header record defines the units for each parameter identified in the second header record. For consistency, the unit mnemonics defined in Table 4.1 or Table 4.4 should be used for all defined parameters. Each unit definition is right justified and aligned beneath the applicable parameter mnemonic in the second header record. The field width is also eight (8) columns for this header record and the units definitions are padded with leading blanks to round up to 8 characters. Unit definitions are required by the 8 column field width definition to be seven (7) characters or less. Fields for variables that do not have associated units, for example CASTNO, are padded with blanks in the third header record. The third header record is padded with blanks at the end until it equals the length of the other header records. If the measurements were converted by the investigator from other units to WOCE units then the conversion method must be referenced or explained quantitatively in the —.DOC file.

- The **fourth** header record defines those parameters in the data record that have associated quality flags in the quality word. Each parameter that has a quality flag associated with it is underlined by seven (7) asterisks preceded by a leading blank so that the column width of each field on this record is eight (8). Parameters that do not have an associated quality flag are padded with blanks on this record and the record is padded with blanks at the end to equal the length of the other header and data records.

One complete record for each water sample observation level on each cast is included in the —.SEA or —.LVS file. The variable type for each parameter is defined in Appendix G under the FORTRAN format column. The field width for each variable in a data record except the quality words (QUALT1 and QUALT2) is eight (8) and each variable and parameter should be right justified in the column beneath its respective mnemonic and units definition in the header records. The quality words are right justified and read with an *m*I1 format where *m* is the number of flags in the quality word and *m* must equal the total number of parameters flagged with asterisks in the fourth header record. A leading blank must exist for the QUALT1 word.

TABLE 4.4: WHP large volume water sample record format description

Column Headings		Units			Reporting Precision	
Parameter* Number	Parameter Mnemonic	Mnemonic	Scientific	Parameter or see note no.	Range	FORTRAN Format
	STNNBR		character	(Note 1)		A8
	CASTNO		integer	(Note 2)		5X,I3
	SAMPNO		character	(Note 3)		1X,A7
	BTLNBR		character	(Note 4)		1X,A7
	THETA	DEG C	°C (ITS_{90})	(Note 5)	–2,35	F8.4
1	***SALNTY***[1]	PSS-78[5]	PSS-78	Salinity[1]	0,42	F8.4
2	***OXYGEN***	UMOL/KG	µmol/kg	Oxygen	0,500	F8.1
	REVPRS	DBAR	decibar	(Note 6)	0,11000	F8.1
	REVTMP[3]	ITS-90	°C (ITS_{90})	(Note 7)	–2,35	F8.3
12	***DELC14***[2]	/MILLE	0/00	^{14}Carbon [2]	–300,250	F8.1
13	***DELC13***[2]	/MILLE	0/00	^{13}Carbon [2]	–5,5	F8.1
14	***KR-85***[2,5]	DM/MG	dpm/1000 kg[4]	^{85}Krypton[2]	0,5	F8.2
15	***ARGON***[2]	UMOL/KG	µmol/kg	Argon[2]	5,25	F8.2
16	***AR-39***[2,5]	PCTMOD	%modern	^{39}Argon[2]	0,100	F8.1
17	***NEON***[2]	NMOL/KG	nmol/kg	Neon[2]	0,10	F8.3
18	***RA-228***[2,5]	DM/.1MG	dpm/100 kg[4]	^{228}Radium[2]	–1,10	F8.2
19	***RA-226***[2,5]	DM/.1MG	dpm/100 kg[4]	^{226}Radium[2]	3,80	F8.2
21	***SR-90***[2,5]	DM/.1MG	dpm/100 kg[4]	^{90}Strontium[2]	0,100	F8.2
22	***CS-137***[2,5]	DM/.1MG	dpm/100 kg[4]	^{137}Cesium[2]	0,100	F8.2
n+1	↓	If the parameter number and mnemonic are not given in Appendix G and an additional number is needed please contact the WHPO for the appropriate number in order to avoid possible conflict with other investigators.				
n+x	↓					
	Parameters requiring conversion factors or expected error data column					
12	C14ERR	/MILLE	0/00	^{14}Carbon[2]		F8.1
13	C13ERR	/MILLE	0/00	^{13}Carbon[2]		F8.1
14	KR85ERR	DM/MG	dpm/1000 kg	^{85}Krypton[2]		F8.2
15	ARGERR	UMOL/KG	nmol/kg	Argon[2]		F8.2
16	AR39ER	PCTMOD	%modern	^{39}Argon[2]		F8.1
17	NEONER	NMOL/KG	nmol/kg	Neon[2]		F8.3
18	R228ER	DM/.1MG	dpm/100 kg[4]	^{228}Radium[2]		F8.2
19	R226ER	DM/.1MG	dpm/100 kg[4]	^{226}Radium[2]		F8.2
	Quality Words					
	QUALT1		none	(Note 8)		*m*I1 + 1
	QUALT2		none	(Note 9)		*m*I1 + 1

One record is required for each Gerard bottle sampled on each cast. The individual water sample records are then compiled into a —.LVS file for submittal to the WHPO. Include only those variables measured during the cruise. All parameters assigned a number and printed in ***BOLD*** *require a quality flag in the quality word.*

Footnotes

* The parameter number defined here and in Appendix G is used in the station summary (—.SUM file, Table 3.5) to identify the measurements made at this station. If no parameter number is defined in Appendix G for a measurement you wish to include please consult with the WHPO.

1 Must use $IPTS_{68}$ for calculating Practical Salinity Scale (PSS-78) until a new algorithm is developed.

2 This parameter requires shore-based analysis that may take up to 18 months.

3 Temperature should always be reported using ITS_{90} temperature scale. If, however, the ITS_{90} scale has not yet been adopted at your institution then it is permissible to report temperature using the $IPTS_{68}$ scale and the WHPO will convert your data to the ITS_{90} scale. If $IPTS_{68}$ scale is used change the mnemonic in the header record to IPTS-68 rather than the default ITS-90 mnemonic.

4 dpm = decays per minute.

5 This mnemonic includes a hyphen (-). Some PIs report machine-dependent problems with the use of hyphens. The WHPO will accept the data with or without a hyphen.

TABLE 4.4: WHP large volume water sample record format description

Notes on Table 4.4

1. A sequential station number (alphanumeric). Station numbers *must* be unique for a cruise but may repeat on subsequent cruises along the same section or to the same station for time series.
2. The cast number: 1 = 1st cast; 2 = 2nd cast on a single station. Every over-the-side operation on a station is given a separate cast number. Cast numbers restart at 1 at each station but are not reset if the same station is visited more than once on the same cruise.
3. The sample number assigned to all water samples drawn from a bottle (alphanumeric). Sample numbers may be unique for a cruise or reflect the position of the bottle on the cast from which the samples were taken. Sample numbers are usually sequential on a cast. In any case *all* groups *must* use the same sample numbering conventions.
4. The permanent, unique serial number of the bottle (alphanumeric) from which the water samples are drawn. Unless a bottle is changed these numbers would usually repeat from cast to cast and station to station.
5. The potential temperature at the time each bottle is tripped. At present it is necessary to calculate initially as theta ($IPTS_{68}$) then convert to theta (ITS_{90}).
6. Pressure as measured by reversing thermometers.
7. The temperature measured by reversing thermometers.
8. The quality word used to identify the quality of the measurement as defined by the investigator. All mnemonics printed in bold and assigned a parameter number require one quality flag each in the quality word for a total of *m* flags, or bytes. The analyst's quality word (QUALT1) always appears as the last variable on the record in the —.LVS file as sent to the WHPO. Note that the bottle number (***BTLNBR***) also has its own independent quality flag defined in Section 4.5.1 on page 52, Table 4.8 and the bottle quality flag is always the first byte of the quality word. Quality flags are optional for non-WOCE parameters.
9. The quality word used to define the quality assurance suggested by the DQE. The DQE quality word (QUALT2) is the last variable in the final data set and is added by the WHPO after submittal of the —.LVS file. The DQE quality check is independent of the chief scientist or cruise participant.

samples are accounted for. After the analysis is completed, the datum is entered in the proper row and column of the —.SEA or —.LVS file and the quality flag for that measurement is reset in the QUALT1 word to the appropriate value as defined in Table 4.9. If water is not drawn for a particular parameter from the water bottle then the quality flag is set to 9.

The QUALT2 word is added by the WHPO after the data are submitted and is used for DQE evaluation.

4.3.3 Header Records For the —.SEA and —.LVS Files

The first four records of the water sample files (—.SEA or —.LVS) are header records. The *first* header record is used to tie the —.SEA file or —.LVS file with the —.SUM file for the cruise. As illustrated in Table 3.7, the first record contains the country-ship code combined with an expedition name (of up to 8 characters) or cruise number and leg (EXPOCODE) as defined in Section 3.3. The WOCE section identification (WHP-ID) is also included together with the cruise dates (MMDDYY) as shown in Table 4.5. If more than one WOCE section or line are occupied during a single leg all section numbers should be included with the WHP-ID, for example, S01, S02, S04, together with any suffixes used to identify subsections. Additional alphanumeric information may be included so long as the fixed record length is not exceeded. The record is then blank padded to the end-of-record (EOR). In the example in Table 4.5 an optional asterisk (*) has been used as an EOR mark.

The *second* header record is composed from the unique mnemonics, defined in Table 4.1 for —.SEA files, Table 4.4 for —.LVS files, or Appendix G, for all variables and parameters measured (or sampled for) on the cruise, including parameters requiring later shore-based

analysis. Each mnemonic is right justified in an eight (8) character field. If a parameter is never measured on a cruise the mnemonic and units are omitted from the header records and the data records following the header are shifted left to fill in the blank. Each mnemonic in the second header record is preceded by leading blanks to pad out the 8-character field width for each variable in the header record except for the quality word QUALT1. QUALT1 is right justified so that it defines the end-of-record (EOR), that is, the 1 in QUALT1 is aligned above the last quality flag in the data records. This ensures that the header records and the data records have the same length.

The *third* header record defines the units of measurement for each parameter defined by the second header record. The units definition is right justified and aligned beneath the applicable parameter mnemonic in the first header record. The field width is also eight (8) characters for this header record. The units definitions are padded with leading blanks to round up to 8 characters. Because of the eight (8) column limitation all unit definitions must be seven (7) characters or less. The unit mnemonics defined in Appendix G (mnemonics for error columns are defined in Table 4.1 or Table 4.4) should be used for all standard parameters to insure consistency between different countries and cruises. Fields for variables that do not have associated units, for example CASTNO, are padded with blanks in the second header record. The third header record is padded with blanks at the end so that the record length is equal to the first header record. If for some reason the units for a parameter are not the standard WOCE units defined in Appendix G, an explanation must be included in the —.DOC file and, if applicable, the quantitative relation of the units given to WOCE units must be defined or referenced.

The *fourth* header record defines those parameters that have associated quality flags in the quality word. Each parameter listed in the second header record that has a quality flag associated with it is underlined by seven (7) asterisks preceded by a leading blank so that the column width of each field on this record is eight (8). Parameters that do not have an associated quality flag are padded with blanks on this record and the record is padded with blanks at the end to equal the length of the other header and data records.

4.3.4 —.SEA and —.LVS File Formatting Notes

All header and data records in the water sample file are kept the same length in order to facilitate direct access read and recording in fixed block format.

The individual data records follow the header records and are vertically aligned and right justified in columns. The field width for each variable in a data record, except the quality words (QUALT1 and QUALT2) is eight (8) columns, and each variable and parameter is right justified in its field beneath the respective mnemonic and units definition in the header records. The quality word is $m + 1$ columns, where m is the number of quality flags for parameters denoted by asterisks in the fourth header record, and the + 1 is a leading blank. There is no upper limit to the number of parameters that can be included in a —.SEA or —.LVS file.

One complete record for each water sample observation level on each cast is included in the —.SEA or —.LVS file. It is suggested that even if a bottle comes up empty that a record be included in the —.SEA or —.LVS files as a placeholder with CTD or reversing thermometer temperature, pressure, salinity, and oxygen included if available.

If a parameter is not measured on a particular cast from a water bottle, or at a given level, the data column(s) are set to –9 and the quality flag is set to 9. Missing data, or shore-based analyses that have not yet been received, are assigned a value of –9 in the data field and a 1, 5, or 9 as appropriate for the quality flag.

The variable type for each parameter is defined in Table 4.1 for the —.SEA file and in Table 4.4 for the —.LVS file under the FORTRAN format column. The FORTRAN format also defines the number of significant figures to be kept for each parameter. Please use a decimal (.) to delineate fractional values rather than a comma (,) and include the leading zero on small numbers, that is, 0.045 rather than .045 or 0,045.

The data records are intended to be read by high level computer languages and consequently only ASCII characters, as shown in Appendix F, should be used. For example, the degree symbol for temperature should not be used in the data files or the header records and U should be substituted for µ (as in UMOL/KG rather than µmol/kg). Upper case, or capital letters should be used exclusively to prevent possible difficulties with case-sensitive programs. The field width for the quality words is a minimum of 8 but can be extended indefinitely with the *m*I1 format (*m* is the number of quality flags in the quality word).

4.3.5 Example —.SEA file

An example of a small volume water sample data set as the WHPO expects to receive it from the chief scientist, that is, without the QUALT2 word, is given in Table 4.5. It is assumed, but not required, that a separate —.SEA file will be prepared for each leg of a multiple leg expedition.

The format for a —.LVS file is the same as shown in Table 4.5 except the parameter mnemonics forming the column headings would follow from Table 4.4 and the CTD parameters would be omitted in most cases.

TABLE 4.5: Example of a merged data set in the —.SEA file

EXPOCODE 99AB123/4 WHP-ID P99 CRUISE DATES 010293 TO 020393 *

STNNBR	CASTNO	SAMPNO	BTLNBR	CTDPRS	CTDTMP	CTDSAL	CTDOXY	THETA	SALNTY	OXYGEN	SILCAT	NITRAT	NITRIT	PHSPHT	CFC-11	QUALT1
				DBAR	ITS-90	PSS-78	UMOL/KG	DEG C	PSS-78	UMOL/KG	UMOL/KG	UMOL/KG	UMOL/KG	PMOL/KG		*
			*******		**********											*
1	1	1	WWA19	2.1	10.1244	33.7425	217.0	10.1242	33.7326	216.7	27.97	22.99	0.22	1.85	1.894	2222222222
1	1	2	WWA20	1.0	9.8955	33.7926	190.3	9.8943	33.7902	190.0	28.66	24.06	0.20	1.92	1.803	2222222222
1	1	3	WWA21	16.3	9.4207	33.8343	173.4	9.4189	33.8177	172.8	30.03	24.74	0.18	1.97	1.720	2222222226
1	1	4	WWA22	41.9	9.0988	33.8850	145.5	9.0943	-9.0000	-9.0	-9.00	-9.00	-9.00	-9.00	-9.000	9229999999
1	1	5	WWA23	66.8	8.8049	33.9302	122.7	8.7979	33.9275	123.1	33.54	27.29	0.20	2.10	-9.000	2222222229
1	1	6	WWA24	92.7	8.6780	33.9873	107.5	8.6683	33.9712	107.0	35.79	27.97	0.24	2.17	1.841	2222222222
2	1	1	WWA19	2.1	10.1959	33.6368	251.0	10.1957	33.6325	251.9	23.50	19.81	0.20	1.54	1.317	3222322223
2	1	3	WWA20	25.6	9.8375	33.6360	231.8	9.8347	33.6207	231.2	24.54	20.58	0.22	1.60	1.808	2222222222
2	1	4	WWA21	51.2	9.2838	33.7728	174.1	9.2783	33.7729	174.5	28.82	23.98	0.27	1.83	1.873	2222222222
2	1	5	WWA22	75.7	8.9514	33.7838	140.0	8.9434	33.7793	140.3	29.50	25.65	0.06	1.90	-9.000	3223333339
2	1	6	WWA23	100.4	8.7613	33.8626	128.5	8.7508	33.8534	127.8	31.73	26.70	0.03	1.96	1.701	2662222228
2	1	7	WWA24	126.2	8.6663	33.9087	121.7	8.6532	33.9027	121.2	33.44	27.26	0.08	2.01	-9.000	2222222229
2	1	8	WWB01	152.1	8.5089	33.9613	17.0	8.4932	33.9487	16.8	36.01	28.08	0.15	2.08	-9.000	2222222229
2	1	9	WWB02	176.5	8.1928	34.0069	103.2	8.1750	33.9967	103.6	39.09	29.22	0.05	2.14	-9.000	2222222229
2	1	10	WWB03	200.6	8.0941	34.0288	102.0	8.0740	34.0174	102.2	40.29	29.66	0.04	2.17	-9.000	4222222229

NOTES:

- Only those parameters sampled during the cruise are included in the —.SEA (or —.LVS) file.
- The —.SEA and —.LVS files are designed to be read by high-level languages such as FORTRAN. Only standard ASCII characters, see Appendix F, are admissible.
- The CTD values are averages taken while the winch is stopped at the time the bottle was tripped. CTD parameters are omitted from —.LVS files or on any cast or cruise that doesn't carry a CTD.
- Quality flag required for mnemonics underlined by asterisks (*). The quality word (QUALT1) is sequentially assembled from the quality flags. Thus, the first byte in the quality word is associated with BTLNBR and the last flag defines CFC11 quality for a total of $m = 11$ flags, or bytes. The second quality word is independently assigned by the DQEs after the —.SEA (or —.LVS) file is submitted to the WHPO. The quality flags are defined in Section 4.5, and are required for all WOCE measurements.

4.4 CTD Format (—.CTD files)

Cruise and position information for each cast are given in the —.SUM file and are cross-referenced with the —.CTD files by EXPOCODE, station number (STNNBR), and cast number (CASTNO). The ASCII file format defined in Table 4.6 should be used when submitting data to the WHPO.

Requirements for precision and accuracy/reproducibility of CTD sensors for the one-time WHP survey are given in Table 2.6 on page 21.

4.4.1 CTD Data

A sample CTD data file is shown in Table 4.7. The first three records contain header information followed by two records containing data column mnemonics and units as defined in Table 4.7. The fifth header record underscores those parameters requiring quality flags in the quality word (QUALT1). All header records should be padded with trailing blanks to make them the same length as the data records. The end-of-record (EOR) characters shown in Table 4.6 and Table 4.7 are optional.

The number of scans indicates the number of observations, or cycles, used to calculate the average temperature, salinity and oxygen at each pressure increment. A description of how the data are averaged, or interpolated, and how pressure measurements are derived, should be included in the —.DOC file.

The quality word consists of quality flags defined in Table 4.10. It is useful to include a description of how you used the quality flags in the —.DOC file.

As shown in Table 4.7, the data recorded by the CTD while it is lowered on station are averaged in standard 2 dbar increments[2] in order of increasing pressure. If the downcast data are not available, the upcast CTD data can be submitted in 2 dbar increments in order of increasing pressure starting at the sea surface (the inverse of the way upcast data are recorded). In the latter event, a note should be placed in the —.DOC file explaining why the downcast data are not available at that station and that the CTD data were recorded while retrieving the CTD.

Additional data observations can be added to each record. Supplementary CTD variables will need appropriate mnemonics and unit descriptions, and detailed descriptions in the —.DOC file. An associated quality flag in the quality word is optional for non-WOCE parameters.

Where noise or other problems create small gaps in the data over several decibars the missing values should be interpolated and flagged with a quality flag of 6. However, interpolation should not be done over large gaps or in regions where conditions are changing rapidly with depth.

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2. A 2 dbar pressure increment is standard but the WHPO will accept data with smaller pressure increments, for example, 1 dbar. Final data from the WHPO, and available from the WHP SAC, will be presented in standard 2 dbar pressure increments.

TABLE 4.6: CTD record format definitions

REC 1 = Country-ship code and cruise/leg designation defined in Section 3.3 plus the WHP-ID, if applicable, for this station. The date (month, day, year, that is, MMDDYY) is also given.
FORMAT('EXPOCODEb',A14,1X,'WHP-IDb',A5,1X,'DATEb',3I2,nX)
where b indicates a blank space and nX indicates blank padding (zero in a standard record) to end of record. Header records are nominally 48 characters long unless parameters in addition to CTDOXY are measured.

REC 2 = Station number and cast number. These variables cross-reference the —.CTD file with the —.SUM file for position, time, etc. The total number of data records in the file is also specified.
FORMAT('STNNBR',A8,1X,'CASTNOb',I3,1X,'NO.bRECORDS=',I5,nX,'2')
To facilitate writing with fixed block format on tape the header records are blank padded (nX in example format) to be the same length as the data records (48 columns for standard CTD cast including oxygen) and the '2' in the example format is optionally used to mark the end-of-record (EOR) with nX blank padding.

REC 3 = Instrument serial number and scans/second of time series data.
FORMAT('INSTRUMENTbNO.b',A5,1X,'SAMPLINGbRATEb',F6.2,'bHZ',nX,'3')
where the '3' is an optional EOR mark with nX blank padding and b is a blank space.

REC 4 = Headers for data columns (variable labels). Example format for *standard* CTD variables:
FORMAT(2X,'CTDPRS',2X,'CTDTMP',2X,'CTDSAL',2X,'CTDOXY',2X,'NUMBER',nX,'QUALT1')
All mnemonic headers, units, and data fields are right justified and eight (8) columns wide except the QUALT1 field. The QUALT1 field must have at least one ($m \geq 1$) leading blank. The 1 in QUALT1 is always the EOR for this header record. If CTD oxygen is not measured the CTDOXY data column should be filled with –9.0 and the quality flag set to 9.

REC 5 = Units headers for data columns. Example format for *standard* CTD variables.
FORMAT(4X,'DBAR',2X,'ITS-90',2X,'PSS-78',1X,'UMOL/KG',4X,'OBS.',nX,'*')
and the '*' is an optional EOR mark with nX blank padding. UMOL/KG is substituted for µmol/kg to facilitate reading with FORTRAN-77 programs and to alleviate possible problems with case-sensitive programs.

REC 6 = Quality flag designators. All parameters requiring a quality flag have their mnemonics underscored by seven (7) asterisks with a leading blank on this record. The field is blank padded for variables without a quality flag. An optional asterisk (*) can be placed in the last column as an EOR mark.
FORMAT(1X,'*******',1X,'*******',1X,'*******',1X,'*******',nX,'*')

REC 7 + NO. RECORDS –1 = Data records: Records through End-of-File (EOF) mark are data observations at odd or even 2 decibar pressure intervals. Data are right justified within an eight (8) column field. The data records are defined in detail below.

Parameter Mnemonic[1]	Units Mnemonic	Units Scientific	Parameter[1]	Reporting Precision Range	Reporting Precision FORTRAN Format
CTDPRS[1]	DBAR	decibar	Pressure	0,11000	F8.1
CTDTMP[1]	ITS-90	°C (ITS_{90})	Temperature	–2,35	F8.4
CTDSAL[1]	PSS-78	PSS-78	Salinity	0,42	F8.4
CTDOXY[1]	UMOL/KG	µmol/kg	Oxygen	0,500	F8.1
XMISS	%TRANS	% light transmitted	Transmissometer	0,100	F8.2
FLUOR	MG/CUM	mg/m^3 (total chlorophyll and phaeopigments)	Fluorescence	0,50	F8.3
—Any additional variables go here.					
NUMBER		integer	Number of scans averaged at this pressure level		I8
QUALT1		none	See note (2)		*m*I1 + 1

NOTES:

1. WOCE parameters are printed in ***BOLD*** and require a quality flag in the quality word. Quality flags are optional for other parameters.
2. The quality word used to identify the quality of the measurement as defined by the investigator. This quality word always appears as the last variable on the CTD data record. The quality word is the left-to-right combination of the required quality flags for the variables measured. For a station where CTDPRS, CTDTMP, CTDSAL, and CTDOXY were measured, the first byte of the quality word relates to CTDPRS and the last flag to CTDOXY. Note that definitions for quality flags for CTD and water sample data may differ. The quality words are read with an *m*I1 format where *m* is the number of flags, or bytes, in the quality word and *m* must equal the total number of parameters flagged with asterisks in the sixth header record. *m* must be at least four (4) and at least one leading blank must exist.

TABLE 4.7: Example of CTD record as submitted to the WHPO

Note that data columns are right justified and aligned beneath their respective header records. Depth interval may be odd or even and could start at 0 or 1 dbar.

EOR
↓

```
EXPOCODE      316N314/2 WHP-ID P16S DATE 052692
STNNBR      18 CASTNO   1 NO. RECORDS= 1500   2
INSTRUMENT NO.   12 SAMPLING RATE 31.00 HZ    3
   CTDPRS  CTDTMP  CTDSAL  CTDOXY  NUMBER QUALT1
     DBAR  ITS-90  PSS-78 UMOL/KG    OBS.      *
 ******* ******* ******* *******             *
     3.0 28.7977 31.8503   209.5      42   2222
     5.0 28.7978 32.0889   208.6       9   2333
     7.0 28.7995 32.3976   210.8      41   2222
     9.0 28.8014 33.0838   212.1      64   2222
    11.0 28.8018 34.6452   199.5     630   2346
    13.0 28.8018 34.4182   198.2      42   2222
    15.0 28.8018 34.4240   202.1      26   2222
    17.0 28.7814 34.4247   202.6      36   2222
    19.0 28.7541 34.4258   199.1      16   2222
    21.0 28.6938 34.4247   190.8     255   2226
    23.0 28.6380 34.4163   193.0      96   2222
    25.0 28.6206 34.4135   193.0      27   2222
    27.0 28.5760 34.4431   197.8      21   2222
    29.0 28.3347 34.5718   203.4      60   2232
    31.0 28.2823 34.5917   197.3     133   2336
    33.0 28.2182 34.5822   199.1      81   2222
    35.0 28.1500 34.6755   203.4     105   2246
    37.0 28.1233 34.5777   201.7      34   2222
```

(and so on to the bottom)

For formatting reasons, a column for CTDOXY should be included even if it is not measured.

4.4.2 CTD Documentation

The CTD documentation provided in the —.DOC file should contain all the information necessary to retrace the processing and calibration steps used to calibrate the CTD sensors, and must address the following issues: List the instruments used during the cruise, any unusual problems, for example, aborted casts, sensor fouling, etc., or special procedures employed during the cruise that would affect data quality, such as cell cleaning, sensor replacements, etc., and specify station numbers affected by these events if applicable. The pre- and post-cruise laboratory calibration information must be included together with the coefficients used to fit CTD pressure and temperature. The conductivity and oxygen calibration coefficients and equations, and the station groups used when fitting to water sample data should also be included. Reference the standard processing procedures employed, or describe variations from these methods and identify the stations on which nonstandard methods were employed. An example of a CTD report is given as part of Appendix C.

4.5 Quality Words

In the diverse and voluminous set of measurements expected during the WOCE Hydrographic Programme, great emphasis is placed on the quality of the data. In order to monitor, evaluate, maintain, and later access the data it is necessary to keep individual records for the quality of each measurement. To accomplish this goal, quality words are used. The bytes in the quality word are flags that define the quality of the measurement they relate to in a machine-readable fashion.

The data are evaluated both by the analyst making the measurement and later, after the data have been submitted to WHPO, by independent data quality evaluators (DQEs) selected by the WHPO. In order to accommodate the quality evaluation of each group, two quality words are used for water samples, one for a self-evaluation by the analyst making the measurement, and a second for the DQEs later, independent evaluation. A DQE quality word is not used with CTD data, however.

4.5.1 Bottle Quality Flags

Each sampling bottle on a cast must be accompanied by a quality flag as defined in Table 4.8.

TABLE 4.8: Quality flag definitions for water bottles.

Flag Value		Definition
1	=	Bottle information unavailable.
2	=	No problems noted.
3	=	Leaking.
4	=	Did not trip correctly.
5	=	Not reported.
6	=	Significant discrepancy in measured values between Gerard and Niskin bottles.
7	=	Unknown problem.
8	=	Pair did not trip correctly. Note that the Niskin bottle can trip at an unplanned depth while the Gerard trips correctly and vice versa.
9	=	Samples not drawn from this bottle.

The bottle quality flag is the first byte of the quality word.

Use of flag 1 is generally limited to non-WOCE or pre-WOCE cruises where bottle information is not available. ***BTLNBR*** is set equal –9 in such data sets. WOCE cruises should use flag 5 if bottle information is not reported.

Flags 6, 7, and 8 apply primarily to large volume samplers.

Note to DQEs: In the QUALT2 word a 1 flag is used as a placeholder when the WHPO creates the QUALT2 word.

The bottle quality flag indicates whether problems were noticed by the observers while drawing samples, or if problems were subsequently determined by the analysts or the DQEs from differences in the measured values. It is critical that questionable bottles be flagged at the earliest possible time.

Because of the unique sampling characteristics of Gerard bottles, which must be tripped simultaneously with a Niskin bottle, additional definitions for the bottle quality flags are required for the large volume samplers. Note that a bottle quality flag of 8 does not necessarily mean a bad sample, just that at least one of the pair of bottles did not trip at the planned depth. Also, the Gerard sampler may trip correctly, and the reversing thermometers on the Niskin bottle work, but the Niskin bottle lid hangs up or for some other reason the Niskin doesn't catch any usable water. In this case the Niskin record would have a ***BTLNBR*** quality flag of 9 and the Gerard barrel would have a quality flag of 8.

4.5.2 Quality Flags for Water Samples

Each water sample measurement is assigned two separate quality flags; the first is generated by the analyst or sample collector for every parameter measured on a cruise, and the second by the DQE. Water sample quality flag definitions are given in Table 4.9. Each

TABLE 4.9: Water sample quality flag definitions.

Flag Value		Definition
1	=	Sample for this measurement was drawn from water bottle but analysis not received. *Note that if water is drawn for any measurement from a water bottle, the quality flag for that parameter must be set equal to 1 initially to ensure that all water samples are accounted for.*
2	=	Acceptable measurement.
3	=	Questionable measurement.
4	=	Bad measurement.
5	=	Not reported.
6	=	Mean of replicate measurements (Number of replicates should be specified in the —.DOC file and replicate data tabulated).
7	=	Manual chromatographic peak measurement.
8	=	Irregular digital chromatographic peak integration.
9	=	Sample not drawn for this measurement from this bottle.

Each water measurement has two quality flags, or bytes, associated with it in two separate quality words. The water quality flags are usually the fourth through *m* flags of the quality words. The definitions here apply both to the analyst and the DQE quality words but not to the CTD (***CTDSAL*** or ***CTDOXY***) parameters or the bottle number (***BTLNBR***).

Note to DQEs: All quality flags in the QUALT2 word are initially set to 1 as a placeholder when the WHPO creates the QUALT2 word.

character within the two quality words flags a bottle number, CTD, or water sample parameter measured on the cruise in the order in which they appear within each data record.

Quality flags are optional for non-WOCE water sample parameters.

The order (left to right) of the characters in each quality word corresponds to the order of the bold mnemonics (top to bottom) recommended in the water sample data files (Table 4.1 or Table 4.4) or the order (left to right) of the variables denoted by asterisks in Table 4.5. If water is drawn for any quality-flagged measurement from a bottle, the quality flag for that parameter must be set equal 1 initially to ensure that all water samples are accounted for. If the parameter is not sampled on a given station, cast, or level the quality flag for that parameter is set to 9.

All measured values should be reported. Questionable or bad values due to sampling, analytical or other problems are flagged but not removed from the data file. Whenever data were expected to be measured from a water sample drawn from a bottle (quality flag = 1), but the observation is missing due to sample loss, contamination, etc., a value of –9 is placed in the measurement field in the data file and the respective quality flag is reset to 5. Quality flags associated with the CTD salinity and CTD oxygen values in the water sample files (—.SEA) can be used to indicate that differences exist between these measurements and the respective water sample observations. The definitions for CTD quality flags, or bytes, given in Table 4.10 in Section 4.4 should be used for these variables. This information is useful in identifying problems with sampling bottles, that is, leaking bottles, pre-trips, etc. Water sample salinity or oxygen values that are not used in the final calibration of the CTD conductivity or oxygen sensors should be flagged with the appropriate quality flag, *not deleted*.

It is not possible to define what is meant by an “acceptable” (quality flag = 2) measurement for all cruises or even all measurements from the same bottle. What may be a questionable, or even bad, measurement on a one time survey may be quite acceptable on some repeat hydrography cruises. Water from the same bottle may be quite adequate for one parameter, for example, salinity, but badly contaminated for another, for example, CFCs. Investigators should be certain that their quality flag assignment for water samples is consistent with the quality flag for the water bottle.

For one time surveys, values that fall appreciably outside the standards defined in Table 2.5 on page 20 should be flagged as questionable (3), or bad (4), as the case may be. Standards for repeat hydrography, including time series, are given in Section 2.1.2 on page 14.

4.5.3 CTD Quality Words

The CTD quality word consists of quality flags defined in Table 4.10. The precision and accuracy/reproducibility required of CTD sensors for the one-time WHP survey are given in Table 2.6 on page 21. Each WOCE CTD parameter has one quality flag, or byte, associated with it in a quality word. Quality flags are optional for non-WOCE parameters. CTD files do not carry a separate DQE quality word.

A CTD quality flag of 1, *not calibrated*, applies to salinity and oxygen measurements only when water samples are collected from the present, or a nearby cast but corrections have not been applied to the CTD data. For pressure and temperature, a quality flag of 1 would indicate final CTD calibrations have not been applied.

TABLE 4.10: Quality flag definitions for CTD data.

Flag Value		Definition
1	=	Not calibrated.
2	=	Acceptable measurement.
3	=	Questionable measurement.
4	=	Bad measurement.
5	=	Not reported.
6	=	Interpolated over >2 dbar interval.
7	=	Despiked.
8		Not assigned for CTD data.
9	=	Not sampled.