

REPORTING FORMAT FOR SEAWATER DATA

TABLE OF CONTENTS

Section	Page
1 OVERVIEW OF THE SEAWATER SYSTEM	1
2 SEAWATER DATA FILE.....	1
2.1 Data file structure.....	1
2.2 Data records included in the seawater formats.....	1
2.3 Depth cycles.....	2
2.4 Linking methods records to data records	3
3 SEAWATER SAMPLE AND SUB-SAMPLE DEFINITIONS	3
3.1 Definitions	3
3.2 Reporting average values	4
3.3 Replicate analyses vs. replicate sub-samples	4
4 DATA ON BIOLOGICAL EFFECTS MEASUREMENTS IN SEAWATER.....	4
4.1 Oyster embryo bioassay	4
4.2 Linking biological effects data and contaminants data	4
5 RECORD LAYOUT DESCRIPTIONS FOR SEAWATER DATA.....	5
5.1 File headers	5
5.2 General field specifications.....	5
5.3 Contaminant Analytical Methods Record (21)	7
5.4 Oyster Embryo Bioassay Methods Record (23).....	8
5.5 Sample Master Record (01)	9
5.6 Parameter/Contaminant Data Record (10).....	10
5.7 Plain Language Comment Record (13).....	11
6 SEAWATER EXAMPLES	12
6.1 Example 1 – Depth cycles (general)	12
6.2 Example 2 – Sub-samples.....	12
6.3 Example 3 – Depth profiles	13
6.4 Example 4 – Duplicate parameter in two sub-sample bottles	13
6.5 Example 5 – Contaminant + oyster embryo bioassay (OEB) data in same sub-sample.....	14
6.6 Example 6 – Contaminant + OEB data in separate sub-samples	14

REPORTING FORMAT FOR SEAWATER DATA

1 OVERVIEW OF THE SEAWATER SYSTEM

The seawater reporting format is used for reporting data on general hydrographic parameters and contaminants (including nutrients) in seawater, and for reporting the results of biological effects measurements using seawater – data type ‘CW’. Although the reporting system is intended to be generally applicable for reporting data on biological effects associated with seawater, it is, at present, only defined for reporting information for the biological effects technique ‘Oyster embryo (seawater) bioassay’.

Each data type has a number of record types associated with it. The record types available for seawater are: The *Contaminant Analytical Methods Record* (RECID: 21), the *Oyster Embryo Bioassay Methods Record* (RECID: 23), the *Sample Master Record* (RECID: 01), the *Contaminant Data Record* (RECID: 10), and the *Plain Language Comment Record* (RECID: 13).

The seawater format description includes sections explaining sample definitions, explanations of data file structure, short descriptions of data record types, sections on the reporting of individual samples, profiles and oyster embryo bioassay data, tables describing layouts for each data record type, and specific examples of the use of the reporting format.

2 SEAWATER DATA FILE

2.1 Data file structure

The data file consists of two parts, the methods section and the results section.

The first section, comprising a series of (one or more) *Contaminant Analytical Methods Records* and/or *Oyster Embryo Bioassay Methods Records*, defines the methods involved in obtaining any particular measurement of a parameter or contaminant in the seawater sample(s). The ‘methods part’ of the data file generally summarizes the methods used by the various laboratories involved in the collection and analysis of the seawater samples in a given year. Reporting institutes are encouraged to pay careful attention to the methods information reported each year, and should not simply assume that the information entered in the previous year’s data file can be repeated. The information reported on the various ‘*Methods Records*’ should form the basis for a historical record of changes in the procedures applied in the monitoring programmes, which is of relevance both in relation to data assessment activities and to the long-term archiving of environmental data.

The second section of the data file includes the actual results of the monitoring activity. This part of the data file comprises a series of (one or more) *Sample Master Records*, each followed by a series of *Parameter/Contaminant Data Records*. Each *Sample Master Record* defines a new seawater sample (station); each *Parameter/Contaminant Data Record* associated with a given *Sample Master Record* details the measurements made for a given parameter in that sample. The *Parameter/Contaminant Data Record* is also used to supplement the ‘sampling occasion’ information found in the master record coordinates by defining a third dimension, the ‘depth’ at which the water sample was taken. By reporting the ‘depth of sampling’ parameter (code DEPH), this record is then used as a *depth cycle* control record (cf. Section 2.3).

Links between the information contained on the *Parameter/Contaminant Data Records* and that contained on the *Contaminant Analytical Methods Records* and/or *Oyster Embryo Bioassay Methods Records* are established using link-keys (cf. Section 2.4).

2.2 Data records included in the seawater formats

The format for reporting data on contaminants and/or biological effects in seawater utilizes the following types of data records:

- The *Contaminant Analytical Methods Record* (RECID: 21)

The *Contaminant Analytical Methods Record* is a general purpose record for recording information on analytical methodologies employed in the contaminant monitoring programmes for seawater, sediment and biota. The record

is used for reporting information on the method of sampling, pretreatment, preservation and analysis for a particular contaminant or parameter by the analytical laboratory involved, for the year concerned. In addition, it includes information on aspects of the laboratory quality assurance programme relevant to the analysis concerned, on the detection limit for the analysis, and on the laboratory's participation in relevant intercomparison exercises. A series of *Contaminant Analytical Methods Records* should be included at the beginning of the data file, describing the methods associated with any contaminant subsequently reported. Each record reports a particular combination of sampling, sample treatment and analytical methods used within a given laboratory for a single contaminant. Thus, the number of records will depend on the number of laboratory-contaminant-sampling-pretreatment-preservation-analysis combinations used in the data being reported. Each contaminant analysis reported later in the data file on a *Parameter/Contaminant Data Record* is unambiguously associated with a specific *Contaminant Analytical Methods Record* by means of an 'Analytical methods link' (AMLNK) identifier.

- The *Oyster Embryo Bioassay Methods Record* (RECID: 23)

The *Oyster Embryo Bioassay Methods Record* is specifically designed for recording information on the method(s) used to obtain oyster embryo bioassay data. The record is used for recording information on the source of the reference seawater used, characteristics of the oysters used, details of the analytical procedure, etc., for the analytical laboratory involved, for the year concerned. In addition, it includes information on aspects of the laboratory quality assurance programme relevant to the bioassay technique. Each bioassay result reported later in the data file on a *Parameter/Contaminant Data Record* is unambiguously associated with a specific *Oyster Embryo Bioassay Methods Record* by means of an 'Analytical methods link' (AMLNK) identifier.

- The *Sample (station) Master Record* (RECID: 01)

The *Sample Master Record* serves as the master record for the series of data deriving from a particular seawater sample, as defined in Section 3.1. The information on a *Sample Master Record* defines a seawater sample in terms of a 'sampling occasion', i.e., it locates the seawater sample in space (sampling area coordinates) and time (sampling date/time) and also supplies administrative information in relation to the intended use of the data.

- The *Parameter/Contaminant Data Record* (RECID: 10)

The *Parameter/Contaminant Data Record* is used for recording data on a range of parameters for the seawater sample. Each record included in the data file is associated with a particular *Sample Master Record* which defines the seawater sample concerned. Each *Parameter/Contaminant Data Record* includes information on a particular parameter or contaminant.

- The *Plain Language Comment Record* (RECID: 13)

Plain Language Comment Records can be inserted at any point in the data file to supply additional information or comments to aid the interpretation of the data reported on the preceding data record. If the explanatory text does not fit on a single *Plain Language Comment Record*, several of these records can be included in a block. It should be noted that, whilst information reported as plain language text will be stored at the data centre, and where possible retrieved and presented together with the data, data handling systems do not generally take account of plain language text. The comments are likely to become dissociated from the coded data, for example during exchange of data in non-ICES format for import into software packages used for data evaluation purposes. Thus, *Plain Language Comment Records* should be avoided unless they are specifically required by the reporting format.

2.3 Depth cycles

The *Parameter/Contaminant Data Records* following any given *Sample Master Record* should be arranged in *depth cycles*, i.e., all records reporting observations at a given sampling depth should be grouped together. The first *Parameter/Contaminant Data Record* following each *Sample Master Record* must always report the parameter 'DEPH' (depth of sampling). Depth of sampling is a mandatory parameter within each *depth cycle* included in the data file; if the depth of sampling is missing, it should either be estimated (and the value qualified accordingly), or the entire set of data for that *depth cycle* should be omitted from the file. See examples in Figure A and Section 6.1.

Figure A is a schematic representation of the data file structure, illustrating the *depth cycle* in the data part of the file.

Figure A – Seawater data file structure

21 or 23 – Analytical or oyster embryo methods recordMETHODS PART
13 – Plain language comment record	
21 or 23 – Analytical or oyster embryo methods record	
:	
01 – Sample (station) master recordDATA PART
13 – Plain language comment record	
10 – Parameter/contaminant data record (PARAM = DEPH)Depth cycle
13 – Plain language comment record	
10 – Parameter/contaminant data record	
:	
10 – Parameter/contaminant data record (PARAM = DEPH)Depth cycle
10 – Parameter/contaminant data record	
:	
01 – Sample (station) master record	
10 – Parameter/contaminant data record (PARAM = DEPH)Depth cycle
10 – Parameter/contaminant data record	
:	
End of file	

2.4 Linking methods records to data records

The seawater data reporting format involves one link-key to relate information items appearing on different data records within the data file:

- The **analytical methods link-key** associates a given measurement (as reported on a particular *Parameter/Contaminant Data Record*) with the information on the methods used to obtain that measurement, as reported on a *Contaminant Analytical Methods Record* or an *Oyster Embryo Bioassay Methods Record*.
The link-key is constructed by concatenating the following data fields, which appear on both the *Contaminant Analytical Methods Records/Oyster Embryo Bioassay Methods Record* and the *Parameter/Contaminant Data Records*:

ALABO + PARAM + AMLNK

The resulting key must be unique for each Analytical Methods Record, whether a *Contaminant Analytical Methods Record* or an *Oyster Embryo Bioassay Methods Record*, included in the data file. The same key can, however, appear on any number of *Parameter/Contaminant Data Records* included in the data file.

3 SEAWATER SAMPLE AND SUB-SAMPLE DEFINITIONS

3.1 Definitions

For the purposes of reporting data using this format, a seawater sample is considered to be all of the ‘water sample(s)’ collected at one sampling station on one sampling occasion. This is, however, not a rigorous definition, and a number of interpretations can be applied depending on the method of collecting water sample(s) and the subsequent handling of the sample(s). To ensure some degree of consistency in the use of the reporting format, the following operational definitions are employed:

- A sample in the context of the seawater reporting format is a ‘**hydrographic station**’ as opposed to an actual water sample; the ‘physical’ water sample (e.g., the seawater collected in an individual bottle) is considered a

‘sub-sample’. The series of data from each station should be reported as a distinct (station) sample under a single *Sample (station) Master Record*.

- Where the station sample consists of several probe measurements or of bottles of seawater, each probe/bottle should be reported as a sub-sample using the ‘Sub-sample number’ (SUBNO) data field on the *Parameter/Contaminant Data Records*.
- ‘Profile’ measurements can be reported using the *depth cycle* structure (cf. Sections 2.3 and 6.1). When several probes/bottles have been taken at the same depth, each should be reported under a separate SUBNO, but within the same *depth cycle*. Within any given *depth cycle*, SUBNO entries are used to associate related values. Thus, the sub-sample concept can be used to positively associate related data, but it can also be used to prevent data association within a given *depth cycle* by reporting a new value under the appropriate sub-sample number (cf. Section 6.4). It is important therefore that, when sub-samples are defined (by entering values in the SUBNO data field), the implications for the record placement on the interpretation of the data are properly appreciated. If any questions arise in relation to this, advice should be sought by contacting ICES.

3.2 Reporting average values

When reporting results for contaminants from a number of sub-sample ‘bottles’, it may be appropriate to simply report a single average value for each contaminant. These average values should also be reported as one sub-sample. However, if the objectives of the monitoring programme require the results to be reported in detail, the ‘sub-sample’ concept must be used to identify and associate data values from a particular water bottle. It is the responsibility of the data originator to ensure that the correct level of detail is available in the information reported; it should be noted that averaged values may subsequently be used in calculations.

3.3 Replicate analyses vs. replicate sub-samples

The purpose of the ‘Replicate number’ (REPNO) data field on the *Parameter/Contaminant Data Record* should be noted. The REPNO field is used to distinguish **replicate analyses** of a given contaminant in a particular ‘analytical sample’, the purpose of which is to provide information on analytical reproducibility. The ‘Sub-sample number’ (SUBNO) data field is used to distinguish **replicate sub-samples**, the purpose of which is to provide information on sampling reproducibility or the homogeneity of the water collected within a given sub-sample. The concepts and purposes of reporting data on a replicate ‘sub-sample’, as identified in the ‘Sub-sample number’ (SUBNO) data field, and data for replicate analyses, as identified in the ‘Replicate number’ (REPNO) data field, should not be confused.

4 DATA ON BIOLOGICAL EFFECTS MEASUREMENTS IN SEAWATER

4.1 Oyster embryo bioassay

The seawater reporting formats incorporate ‘oyster embryo bioassay’ measurements by using the parameter ‘percent net response’ (PNR). The only modification to the reporting format for contaminants in seawater, when using it to report oyster embryo bioassay data, involves the inclusion of an additional record type. This record, the *Oyster Embryo Bioassay Methods Record*, is used to describe the methods employed to obtain the bioassay results. One (or more) of these records are placed in the ‘methods part’ of the data file after the *Contaminant Analytical Methods Records*, if any.

When reporting oyster embryo bioassay data, a number of items of information appearing on the various data records, which may be optional in the context of reporting contaminants data, are considered mandatory. The *Oyster Embryo Bioassay Methods Record* defines data fields for information concerning the methodology employed. On the *Sample Master Record*, the ‘Water depth’ (WADEP) should be recorded. In each *depth cycle* including oyster embryo bioassay results, the parameters ‘Dissolved oxygen’ (DOXY), ‘Hydrogen ion concentration’ (pH), and ‘Chlorophyll-a’ (CPHL) should be reported in addition to the mandatory parameters sampling depth, temperature, salinity and suspended solids.

4.2 Linking biological effects data and contaminants data

An important consideration in relation to biological effects data is the ability to compare them with chemistry data in order to correlate results. To achieve this, it is necessary to consider mechanisms for ‘linking’ water samples analysed for biological effects with appropriate contaminants data. In the case of the oyster embryo bioassay, it is only appropriate to relate bioassay data with data on contaminants measured in the same water sample or in a water sample taken in parallel at the same point in space and time.

(i) When the same water sample bottle is used for both biological effects measurements and contaminant analyses, all data are reported under the same ‘Sub-sample number’ (SUBNO) in the *Parameter/Contaminant Data Records* which are included in a given *depth cycle*. This combination of data is reported as shown in Example 5 in Section 6.5.

(ii) Where the oyster embryo bioassay data and the data for contaminants are measured in different water sample bottles collected at the same location and at the same depth and time, with a view to subsequent comparison of the two sets of information, they are reported as illustrated in Example 6 in Section 6.6. Although the data are associated with different ‘Sub-sample numbers’ (SUBNOs), the ‘link’ is formed by the fact that both water samples are reported under the same *depth cycle*.

5 RECORD LAYOUT DESCRIPTIONS FOR SEAWATER DATA

5.1 File headers

The first record of every file must be a file header, i.e., a 00-record, specifying the version numbers of the reporting format, the screening program, and the valid code list file (for example: **00 RF2.2 SV1.34 LR1**). The header numbers should coincide with the latest updates

5.2 General field specifications

The following sections describe the layout of each record type found in the seawater data reporting format. Each record is presented in the form of a table where the following are described for each data field of the record: the data field code, the data field name, the field column numbers, the valid values for the field, the format for the field, and whether the field is mandatory.

The data **field codes** and the data **field names** are described in detail in the section on Data Field Descriptions of this manual.

The **column** numbers refer to the column placement of the field in a given record.

The **valid values** for the field describe predefined values and ranges, and refer to Environmental reference codes found on the web at www.ices.dk/env/ (choose Codes).

The **format** column for the field indicates the type of variable included in the indicated data field according to one of the following:

SPC n a ‘space filled’ character field, consisting of n spaces.

CHAR n a character field of n characters. Character fields are formatted as left-justified, space filled.

NUM n a numeric (integer) field of width n . Integer fields are formatted as right justified, zero filled – e.g., the number 43 in a field NUM4:

0	0	4	3
---	---	---	---

NUM n m a numeric field of width n , including an **implied** decimal point; the rightmost m positions in the field are decimal positions. Values are formatted as decimal justified, zero filled — e.g., the number 3.7 in a field NUM4i2:

0	3.	7	0
---	----	---	---

NUM n m a numeric field of width n , including an **exponent**: the mantissa occupies the leftmost $n - 4$ positions, including an implied decimal point; the rightmost m positions in the mantissa are decimal positions. The exponent occupies the rightmost 4 positions (‘E±dd’); Values are formatted as decimal justified, space filled – e.g., the number 56.1 in a field NUM9e4:

5.	6	1			E	+	0	1
----	---	---	--	--	---	---	---	---

The **mandatory**, or ‘M’, column indicates those data fields which are mandatory in the context of the reporting formats, i.e., data which **must be reported**; the following codes apply:

- m mandatory;
- m? mandatory in some cases, e.g., when reporting data for a specific programme;
- mH mandatory when reporting data to HELCOM (BMP/COMBINE);
- mO mandatory when reporting data to OSPARCOM (JMP/JAMP);
- x mandatory and predefined (i.e., insert the characters specified in the valid values column).

5.3 Contaminant Analytical Methods Record (21)

RECORD: Contaminant Analytical Methods Record					
Code	Field name	Columns	Valid values	Format	M
RECID	Record identifier	1–2	‘21’	NUM2	x
DTYPE	Data type	3–4	‘CW’	CHAR2	x
RLABO	Reporting institute code	5–8	cf. RLABO	CHAR4	m
ALABO	Analytical laboratory code	9–12	cf. RLABO	CHAR4	m
MYEAR	Monitoring year	13–14	‘74’ to present year	NUM2	m
PARAM	Parameter code	15–19	cf. PARAM	CHAR5	m
AMLNK	Analytical methods link	20–21	01–99	NUM2	m
METSW	Method of sampling seawater	22–23	A–z, 0–9	CHAR2	m
METPT	Method of separation of solids / pretreatment of seawater samples	24–25	A–z, 0–9 or spaces	CHAR2	
METEX	<i>Field not used in seawater data</i>	26–29	spaces	SPC4	x
COSED	<i>Field not used in seawater data</i>	30–30	spaces	SPC1	x
METSP	Method of storage / preservation of sample	31–32	A–z, 0–9	CHAR2	m
METAN	Method of analysis of parameter / contaminant	33–35	A–z, 0–9	CHAR3	m
DETLB	<i>Field not used in seawater data</i>	36–36	space	SPC1	x
DETLI	Detection limit value	37–45	–0000 to 99999 plus ‘E’ plus –99 to +99	NUM9e4	m
ICCOD	Intercomparison exercise code	46–47	cf. ICCOD	CHAR2	m?
	Control chart information				
CONCH	Control chart basis	48–50	cf. CONCH and. Data Field Descriptions	CHAR3	mO
CRMCO	Control chart reference material code	51–58	cf. CRMCO and Data Field Descriptions	CHAR8	mO
CRMMB	<i>Field not used in seawater data</i>	59–59	space	SPC1	x
CRMMV	Control chart RM mean value – value	60–68	–0000 to 99999 plus ‘E’ plus –99 to +99, or spaces	NUM9e4	mO
CRMSD	Control chart reference material – standard deviation	69–77	–0000 to 99999 plus ‘E’ plus –99 to +99, or spaces	NUM9e4	mO
CRMNM	Control chart reference material – number of measurements	78–79	01–99 or spaces	NUM2	mO
CRMPE	Control chart reference material – period	80–81	01–99 or spaces	NUM2	mO
RBMEA	Robust mean	82–90	–0000 to 99999 plus ‘E’ plus –99 to +99, or spaces	NUM9e4	
ZSCOR	Z-score	91–99	–0000 to 99999 plus ‘E’ plus –99 to +99, or spaces	NUM9e4	
PSCOR	P-score	100–108	–0000 to 99999 plus ‘E’ plus –99 to +99, or spaces	NUM9e4	
		109–120	spaces	SPC	x

5.4 Oyster Embryo Bioassay Methods Record (23)

RECORD: Oyster Embryo Bioassay Methods Record					
Code	Field name	Columns	Valid values	Format	M
RECID	Record identifier	1–2	'23'	NUM2	x
DTYPE	Data type	3–4	'CW'	CHAR2	x
RLABO	Reporting institute code	5–8	cf. RLABO	CHAR4	m
ALABO	Analytical laboratory code	9–12	cf. RLABO	CHAR4	m
MYEAR	Monitoring year	13–14	'74' to present year	NUM2	m
PARAM	Parameter code	15–19	'PNR' (cf. PARAM)	CHAR5	m
AMLNK	Analytical methods link	20–21	01–99	NUM2	m
OELWA	<i>Field not used in seawater data</i>	22–22	spaces	SPC1	x
VOLRA	<i>Field not used in seawater data</i>	23–25	spaces	SPC3	x
DUREL	<i>Field not used in seawater data</i>	26–27	spaces	SPC2	x
METOB	Method of oyster embryo bioassay	28–30	'T11', A–z or 0–9	CHAR3	m
SPECI	Species (RUBIN) code	31–38	cf. SPECI	CHAR8	m
OOYST	Origin of oysters	39–40	cf. OOYST	CHAR2	m
MOYST	Month of collecting oysters	41–42	01–12	NUM2	m
COYST	Conditioning of oysters	43–43	'Y' or 'N'	CHAR1	m
SREFW	Source of reference seawater	44–44	cf. SREFW	CHAR1	m
MWTOY	Mean live weight of oysters (g)	45–47	001–999	NUM3	m
NUMCR	Number of control replicates	48–49	01–99	NUM2	m
NUMSR	Number of sample replicates	50–51	01–99	NUM2	m
VEGGS	Volume of egg suspension (ml)	52–54	001–999	NUM3i1	m
AEREP	Aeration of replicates	55–55	'Y' or 'N'	CHAR1	m
DURSE	Duration of storage of embryos	56–58	001–999 or spaces	NUM3	
		59–120	spaces	SPC	x

5.5 Sample Master Record (01)

RECORD: Sample Master Record					
Code	Field name	Columns	Valid values	Format	M
RECID	Record identifier	1–2	'01'	NUM2	x
DTYPE	Data type	3–4	'CW'	CHAR2	x
RLABO	Reporting institute code	5–8	cf. RLABO	CHAR4	m
MYEAR	Monitoring year	9–10	'74' to present year	NUM2	m
SEQNO	Sample sequence number	11–14	0001–9999	NUM4	m
CNTRY	Country code	15–16	cf. CNTRY	CHAR2	m
SHIPC	Ship code	17–18	cf. SHIPC	CHAR2	m
CRUIS	Cruise identifier	19–22	A–z, 0–9	CHAR4	m
SDATE	Sampling date	23–28	000000–999999	CHAR6	m
STIME	Sampling time	29–32	0000–2359 or spaces	CHAR4	
	Sampling area coordinates				
LATDG	Latitude degrees	33–34	00–90 (north)	NUM2	m
LATMI	Latitude minutes	35–36	00–59	NUM2	m
LATMF	Latitude decimal minutes	37–38	00–99	NUM2	m
LONDG	Longitude degrees	39–40	00–99	NUM2	m
LONMI	Longitude minutes	41–42	00–59	NUM2	m
LONMF	Longitude decimal minutes	43–44	00–99	NUM2	m
QEORW	Quadrant	45–45	'E', 'e', 'W' or 'w' (cf. Data Field Descriptions)	CHAR1	m
JMPAR	JMP area code	46–54	cf. JMPAR and Data Field Descriptions, or spaces	CHAR9	mO
ICEAR	ICES statistical rectangle	55–59	cf. ICEAR	CHAR5	m
OTHAR	Other area or station code	60–64	A–z, 0–9 or spaces	CHAR5	mH
SPECI	<i>Field not used in seawater data</i>	65–72	spaces	SPC8	x
NOINS	<i>Field not used in seawater data</i>	73–75	spaces	SPC3	x
WADEP	Water depth	76–79	0000–9999 or spaces	NUM4	m?
COREL	<i>Field not used in seawater data</i>	80–82	spaces	SPC3	
ESTSR	<i>Field not used in seawater data</i>	83–85	spaces	SPC3	
SMLNK	<i>Field not used in seawater data</i>	86–87	spaces	SPC2	
ORGNZ	Organization codes	88–92	cf. ORGNZ	CHAR5	m
PURPM	Purpose of monitoring codes	93–97	cf. PURPM	CHAR5	m
RLIST	<i>Field not used in seawater data</i>	98–99	spaces	SPC2	x
VESSL	Vessel type	100–100	cf. VESSL	CHAR1	m
GEART	<i>Field not used in seawater data</i>	101–103	spaces	SPC3	x
NOHAU	<i>Field not used in seawater data</i>	104–105	spaces	SPC2	x
SPSEA	<i>Field not used in seawater data</i>	106–106	spaces	SPC1	x
TOTIN	<i>Field not used in seawater data</i>	107–110	spaces	SPC4	x
ASTSA	<i>Field not used in seawater data</i>	111–111	spaces	SPC1	x
STTYP	Station type	112–112	cf. STTYP	CHAR1	m
PTSRC	Point source of contamination	113–113	cf. PTSRC	CHAR1	
		114–120	spaces	SPC	x

5.6 Parameter/Contaminant Data Record (10)

RECORD: Parameter/Contaminant Data Record					
Code	Field name	Columns	Valid values	Format	M
RECID	Record identifier	1–2	'10'	NUM2	x
DTYPE	Data type	3–4	'CW'	CHAR2	x
RLABO	Reporting institute code	5–8	cf. RLABO	CHAR4	m
MYEAR	Monitoring year	9–10	'74' to present year	NUM2	m
SEQNO	Sample sequence number	11–14	0001–9999	NUM4	m
INORB	<i>Field not used in seawater data</i>	15–15	space	SPC1	x
SUBNO	Sub-sample number	16–17	01–99	NUM2	m
	<i>Field reserved</i>	18–25	spaces	SPC8	x
MATRX	Matrix analysed	26–27	cf. MATRX and Data Field Descriptions	CHAR2	m
PARAM	Parameter code	28–32	cf. PARAM	CHAR5	m
VFLAG	Validity flag	33–33	cf. VFLAG	CHAR1	
QFLAG	Qualifier flag	34–34	'<' or space	CHAR1	
VALSN	Value in scientific notation	35–43	–0000 to 99999 plus 'E' plus –99 to +99	NUM9e4	m
BASIS	<i>Field not used in seawater data</i>	44–44	spaces	SPC1	x
SFRAC	<i>Field not used in seawater data</i>	45–48	spaces	SPC4	x
REPNO	Replicate number	49–50	01–99 or spaces	NUM2	
PERCR	<i>Field not used in seawater data</i>	51–54	spaces	SPC4	x
AMLNK	Analytical methods link	55–56	01–99	NUM2	m
ALABO	Analytical laboratory code	57–60	cf. RLABO	CHAR4	m
		61–120	spaces	SPC	x

5.7 Plain Language Comment Record (13)

RECORD: Plain Language Comment Record					
Code	Field name	Columns	Valid values	Format	M
RECID	Record identifier	1-2	'13'	NUM2	x
PTEXT	Plain text	3-87		CHAR85	
		88-120	spaces	SPC	x

6 SEAWATER EXAMPLES

6.1 Example 1 – Depth cycles (general)

Seawater samples are taken at 0 m (nominal surface sample), 10 m, and 30 m, respectively, and analysed for contaminants and hydrographic parameters. The arrangement of records in the ‘data part’ of the data file would be as follows:

01–Sample master record (defines a sample/sampling occasion)

10 – Data record for sampling depth	(PARAM = DEPH ; VALSN = 0E+00; SUBNO = 01)
10 – Data record for temperature, at depth 0 m	(PARAM = TEMP; SUBNO = 01)
10 – Data record for salinity, at depth 0 m	(PARAM = PSAL; SUBNO = 01)
:	
10 – Data record for contaminant P1, at depth 0 m	(PARAM = P1; SUBNO = 01)
10 – Data record for contaminant P2, at depth 0 m	(PARAM = P2; SUBNO = 01)
:	
10 – Data record for sampling depth	(PARAM = DEPH ; VALSN = 1E+01; SUBNO = 02)
10 – Data record for temperature, at depth 10 m	(PARAM = TEMP; SUBNO = 02)
10 – Data record for salinity, at depth 10 m	(PARAM = PSAL; SUBNO = 02)
:	
10 – Data record for contaminant P1, at depth 10 m	(PARAM = P1; SUBNO = 02)
10 – Data record for contaminant P2, at depth 10 m	(PARAM = P2; SUBNO = 02)
:	
10 – Data record for sampling depth	(PARAM = DEPH ; VALSN = 3E+01; SUBNO = 03)
10 – Data record for temperature, at depth 30 m	(PARAM = TEMP; SUBNO = 03)
10 – Data record for salinity, at depth 30 m	(PARAM = PSAL; SUBNO = 03)
:	
10 – Data record for contaminant P1, at depth 30 m	(PARAM = P1; SUBNO = 03)
10 – Data record for contaminant P2, at depth 30 m	(PARAM = P2; SUBNO = 03)
:	

6.2 Example 2 – Sub-samples

At a particular station, seawater samples are collected from one depth. Two bottles are collected for the analysis of trace metals and nutrients, respectively. Temperature (TEMP) and salinity (PSAL) are measured by a probe, i.e., the values for these two parameters are not directly associated with either of the two bottle ‘sub-samples’. In the reporting of these results, a possible misinterpretation of the data could arise if these results were reported with the ‘trace metals sub-sample’ but not with the ‘nutrients sub-sample’ data. In order to avoid such an interpretation, the TEMP and PSAL data records should be reported as a separate ‘sub-sample’ with a separate SUBNO value (here as SUBNO ‘01’). The placement of the values as SUBNO ‘01’ within the same *depth cycle* as the trace metals and the nutrients ensures that these values will be associated with both the trace metals sub-sample (SUBNO ‘02’) and the nutrients sub-sample (SUBNO ‘03’).

01 – Sample master record (defines a sample/sampling occasion)

- 10 – Data record for sampling depth (PARAM = **DEPH**; SUBNO = **01**)
- 10 – Data record for temperature (PARAM = TEMP; SUBNO = 01)
- 10 – Data record for salinity (PARAM = PSAL; SUBNO = 01)
- 10 – Data record for trace metal P1 (PARAM = P1; SUBNO = **02**)
- 10 – Data record for trace metal P2 (PARAM = P2; SUBNO = 02)
- 10 – Data record for trace metal P3 (PARAM = P3; SUBNO = 02)
- 10 – Data record for nutrient P4 (PARAM = P4; SUBNO = **03**)
- 10 – Data record for nutrient P5 (PARAM = P5; SUBNO = 03)

6.3 Example 3 – Depth profiles

In example 2 above, results from only one depth were reported. In this example, a depth profile is made and TEMP, PSAL, trace metals and nutrients are measured within each depth level. Each probe and sub-sample are reported as separate sub-samples with different SUBNOs and within an appropriate *depth cycles* structure.

01 – Sample master record (defines a sample/sampling occasion)

- 10 – Data record for sampling depth (PARAM = **DEPH**; SUBNO = **01**)
- 10 – Data record for temperature (PARAM = TEMP; SUBNO = 01)
- 10 – Data record for salinity (PARAM = PSAL; SUBNO = 01)
- 10 – Data record for trace metal P1 (PARAM = P1; SUBNO = 02)
- 10 – Data record for trace metal P2 (PARAM = P2; SUBNO = 02)
- 10 – Data record for trace metal P3 (PARAM = P3; SUBNO = 02)
- 10 – Data record for nutrient P4 (PARAM = P4; SUBNO = 03)
- 10 – Data record for nutrient P5 (PARAM = P5; SUBNO = 03)
- 10 – Data record for sampling depth (PARAM = **DEPH**; SUBNO = **04**)
- 10 – Data record for temperature (PARAM = TEMP; SUBNO = 04)
- 10 – Data record for salinity (PARAM = PSAL; SUBNO = 04)
- 10 – Data record for trace metal P1 (PARAM = P1; SUBNO = **05**)
- 10 – Data record for trace metal P2 (PARAM = P2; SUBNO = 05)
- 10 – Data record for trace metal P3 (PARAM = P3; SUBNO = 05)
- 10 – Data record for nutrient P4 (PARAM = P4; SUBNO = **06**)
- 10 – Data record for nutrient P5 (PARAM = P5; SUBNO = 06)
- 10 – Data record for sampling depth (PARAM = **DEPH**; SUBNO = **07**)
- :
- 10 – Data record for trace metal P1 (PARAM = P1; SUBNO = **08**)
- :
- 10 – Data record for nutrient P4 (PARAM = P4; SUBNO = **09**)

6.4 Example 4 – Duplicate parameter in two sub-sample bottles

Compared to example 2 above, an additional parameter has now been included. SUBNO ‘02’ is now being used for the analysis of trace metals and suspended particulate matter (SPM), and SUBNO ‘03’ is being used for the analysis of nutrients and SPM. Due to different methods employed to separate suspended particulates, the amounts of ‘suspended solids (SPM)’ measured in the two bottles differ.

In the reporting of the results, both values for SPM are reported (as results for the parameter ‘SUSP’). It is important to distinguish between the two SPM values so that, e.g., in a calculation of trace metal loadings, the SPM value used in the calculation is that associated with the trace metal concentration values and not that derived from the nutrient water bottle.

01 – Sample master record (defines a sample/sampling occasion)

10 – Data record for sampling depth	(PARAM = DEPH ; SUBNO = 01)
10 – Data record for temperature	(PARAM = TEMP; SUBNO = 01)
10 – Data record for salinity	(PARAM = PSAL; SUBNO = 01)
10 – Data record for suspended solids	(PARAM = SUSP ; SUBNO = 02)
10 – Data record for trace metal P1	(PARAM = P1; SUBNO = 02)
10 – Data record for trace metal P2	(PARAM = P2; SUBNO = 02)
10 – Data record for trace metal P3	(PARAM = P3; SUBNO = 02)
10 – Data record for suspended solids	(PARAM = SUSP ; SUBNO = 03)
10 – Data record for nutrient P4	(PARAM = P4; SUBNO = 03)
10 – Data record for nutrient P5	(PARAM = P5; SUBNO = 03)

6.5 Example 5 – Contaminant + oyster embryo bioassay (OEB) data in same sub-sample

Seawater samples are taken at 0 m (nominal surface sample) and 10 m, and analysed for hydrographic parameters, contaminants, and the oyster embryo bioassay (OEB). One sample is taken per depth level. The arrangement of records in the ‘data part’ of the data file would be as follows:

01 – Sample master record (defines a sample/sampling occasion)

10 – Data record for sampling depth	(PARAM = DEPH ; SUBNO = 01)
10 – Data record for temperature, at depth 0 m	(PARAM = TEMP; SUBNO = 01)
10 – Data record for salinity, at depth 0 m	(PARAM = PSAL; SUBNO = 01)
:	
10 – Data record for contaminant P1, at depth 0 m	(PARAM = P1; SUBNO = 01)
10 – Data record for contaminant P2, at depth 0 m	(PARAM = P2; SUBNO = 01)
:	
10 – Data record for OEB results, at depth 0 m	(PARAM = PNR; SUBNO = 01)
:	
10 – Data record for sampling depth	(PARAM = DEPH ; SUBNO = 02)
10 – Data record for temperature, at depth 10 m	(PARAM = TEMP; SUBNO = 02)
10 – Data record for salinity, at depth 10 m	(PARAM = PSAL; SUBNO = 02)
:	
10 – Data record for contaminant P1, at depth 10 m	(PARAM = P1; SUBNO = 02)
10 – Data record for contaminant P2, at depth 10 m	(PARAM = P2; SUBNO = 02)
:	
10 – Data record for OEB results, at depth 10 m	(PARAM = PNR; SUBNO = 02)
:	

6.6 Example 6 – Contaminant + OEB data in separate sub-samples

Measurements are reported for seawater samples taken at 0 m (nominal surface sample); temperature and salinity are determined by a probe. Three bottle samples are taken, one is used for determining suspended solids, dissolved oxygen and chlorophyll-a, the second for contaminants and suspended solids, and the third for the oyster embryo bioassay (OEB) and suspended solids. The arrangement of records in the ‘data part’ of the data file would be as follows:

01 – Sample master record (defines a sample/sampling occasion)

10 – Data record for sampling depth	(PARAM = DEPH ; SUBNO = 01)
10 – Data record for temperature	(PARAM = TEMP; SUBNO = 01)
10 – Data record for salinity	(PARAM = PSAL; SUBNO = 01)

10 – Data record for suspended solids	(PARAM = SUSP; SUBNO = 02)
10 – Data record for dissolved oxygen	(PARAM = DOXY; SUBNO = 02)
10 – Data record for chlorophyll-a	(PARAM = CPHL; SUBNO = 02)
10 – Data record for suspended solids	(PARAM = SUSP; SUBNO = 03)
10 – Data record for contaminant P1	(PARAM = P1; SUBNO = 03)
10 – Data record for contaminant P2	(PARAM = P2; SUBNO = 03)
10 – Data record for contaminant P3	(PARAM = P3; SUBNO = 03)
10 – Data record for suspended solids	(PARAM = SUSP; SUBNO = 04)
10 – Data record for oyster embryo bioassay	(PARAM = PNR; SUBNO = 04; REPNO = 1)
10 – Data record for oyster embryo bioassay	(PARAM = PNR; SUBNO = 04; REPNO = 2)
10 – Data record for oyster embryo bioassay	(PARAM = PNR; SUBNO = 04; REPNO = 3)
10 – Data record for oyster embryo bioassay	(PARAM = PNR; SUBNO = 04; REPNO = 4)
:	

The oyster embryo bioassay ‘Percent net response’ (PNR) measurements are reported for four replicate determinations using water from the same sample bottle (SUBNO 04), identified by the REPNO entries (1–4). Although the first sample bottle was taken for suspended solids, dissolved oxygen and chlorophyll-a, since the latter two measurements are not repeated for other sample bottles, they will be considered general parameters. Thus, the dissolved oxygen and chlorophyll-a parameters may be related to the oyster embryo bioassay results. The suspended solids value reported in SUBNO ‘03’ is, however, superseded by the suspended solids value for SUBNO ‘04’, i.e., the ‘SUSP’ value directly associated with the bioassay sample.