### CARBON DIOXIDE, HYDROGRAPHIC, AND CHEMICAL DATA OBTAINED DURING THE R/V METEOR CRUISE 18/1 IN THE NORTH ATLANTIC OCEAN (WOCE SECTION A1E, SEPTEMBER 1991)

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## ABSTRACT

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The North Atlantic Ocean is characterized by an intense meridional circulation cell carrying near-surface waters of tropical and subtropical origin northward and deep waters of arctic and subarctic origin southward. The related "overturning" is driven by the sinking of water masses at high latitudes. The overturning rate and thus the intensity of the meridional transports of mass, heat, and salt, is an important control parameter for the modeling of the ocean's role in climate. Certainly such estimates require more than one survey of the study area; therefore, the Research Vessel (R/V) *Meteor* Cruise 18/1 was one in a series of cruises in the North Atlantic that started in March 1991 and continued until 1995 (Meincke 1993).

This data documentation discusses the procedures and methods used to measure total carbon dioxide (TCO<sub>2</sub>) and total alkalinity (TALK) at hydrographic stations, as well as underway partial pressure of CO<sub>2</sub> (pCO<sub>2</sub>) measured during the R/V Meteor Cruise 18/1 in the North Atlantic Ocean (Section A1E). Conducted as part of the World Ocean Circulation Experiment (WOCE) and the German North Atlantic Overturning Rate Determination expedition, the cruise began in Reykjavik, Iceland, on September 2, 1991, and ended after 24 days at sea in Hamburg, Germany, on September 25, 1991. WOCE Zonal Section A1E began at 60° N and 42°30' W (southeast of Greenland) and continued southeast with a closely spaced series of hydrocasts to 52°20' N and 14°15' W (Porcupine Shelves). Measurements made along WOCE Section A1E included pressure, temperature, salinity, and oxygen measured by a conductivity, temperature and depth (CTD) sensor; bottle salinity; oxygen; phosphate; nitrate; nitrite; silicate; TCO<sub>2</sub>; TALK; and underway pCO<sub>2</sub>. A total of 61 CTD casts were made, including 59 bottle casts and 2 calibration stations. Replicate samples from seven Niskin bottles at five stations were also collected for later shorebased reference analyses of TCO<sub>2</sub> by vacuum extraction and manometry and TALK in the laboratory of Dr. Charles D. Keeling, Scripps Institution of Oceanography; these results are also included in this report.

TCO<sub>2</sub> was measured by using an automated sample processor, to extract CO<sub>2</sub> from seawater samples, coupled to a coulometer, to detect the extracted gas. The precision and accuracy of the system was  $\pm 1.60 \ \mu mol/kg$ . Samples collected for TALK were measured using standard potentiometric techniques; precision was  $\pm 2.0 \ \mu mol/kg$ . Underway pCO<sub>2</sub> was measured by infrared photometry; precision was  $\pm 2 \ \mu atm$ .

The R/V *Meteor* Cruise 18/1 data set is available free of charge as a numeric data package (NDP) from the Carbon Dioxide Information Analysis Center. The NDP consists of three oceanographic data files, three FORTRAN 77 data retrieval routine files, a readme file, and this printed documentation, which describes the contents and format of all files as well as the procedures and methods used to obtain the data.

**Keywords:** carbon dioxide; alkalinity, pCO<sub>2</sub>, World Ocean Circulation Experiment; North Atlantic Ocean; hydrographic measurements; carbon cycle

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# PART 1:

## **OVERVIEW**

## **1. BACKGROUND INFORMATION**

To better understand the ocean's role in climate and climatic changes, several large experiments have been conducted in the past, and others are currently under way. The World Ocean Circulation Experiment (WOCE) is a major component of the World Climate Research Program. Although total carbon dioxide (TCO<sub>2</sub>) is not an official WOCE measurement, a coordinated effort, supported in the United States by the U.S. Department of Energy (DOE) and the National Oceanic and Atmospheric Administration, is being made on WOCE cruises to measure the global, spatial, and temporal distributions of TCO<sub>2</sub> and other carbon-related parameters. The CO<sub>2</sub> survey goals include estimation of the meridional transport of inorganic carbon in a manner analogous to the oceanic heat transport (Bryden and Hall 1980; Brewer et al. 1989; Roemmich and Wunsch 1985), evaluation of the exchange of CO<sub>2</sub> between the atmosphere and the ocean, and preparation of a database suitable for both carbon-cycle modeling and the subsequent assessment of the anthropogenic CO<sub>2</sub> increase in the oceans. The final data set is expected to cover ~23,000 stations in the Atlantic, Pacific, and Indian oceans.

The Research Vessel (R/V) *Meteor* Cruise 18/1, from Reykjavik, Iceland, to Hamburg, Germany, from September 2 to 25, 1991, completed WOCE Zonal Section A1E (Fig. 1). It was one of a series of cruises starting in 1991 that are contributing to the WOCE North Atlantic Overturning Rate Determination (WOCE-NORD) program. The WOCE-NORD program is coordinated jointly by the Bundesamt für Seeschiffahrt und Hydrographie (Hamburg) and the Institut für Meereskunde (Hamburg). The sampling strategy of WOCE-NORD is to combine seasonally repeated hydrographic sections between southern Greenland and Iceland with current measurements from moored arrays. Program objectives include the direct determination of the overturning rates and the intensity of the meridional transports of mass, heat, and salt. Section A1E was chosen to be south of the major wintertime convection regions so as to avoid both water mass formation processes and shallow topography, either of which could cause difficulties in calculating volume transports.

This document describes the cooperative efforts of chemical oceanographers from Brookhaven National Laboratory (BNL) and the Institut für Meereskunde Kiel (IFMK) to make high-quality  $CO_2$  measurements along the WOCE Section A1E.

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Figure 1. Station locations during R/V Meteor Cruise 18/1 (WOCE Section A1E).

## 2. DESCRIPTION OF THE RESEARCH VESSEL AND EXPEDITION

### 2.1 R/V Meteor: Technical Details and History

The R/V *Meteor* is owned by the Federal Republic of Germany's Ministry of Research and Technology (BMFT), which financed its construction. It is operated by the German Research Foundation (DFG), which provides about 70% of its operating funds while BMFT supplies the remainder. DFG also plans the scientific cruises and appoints the chief scientists. The Operations Control Office of the University of Hamburg is responsible for management, logistics, execution, and supervision of ship operations. These functions are performed through cooperation with expedition coordinators and the managing owners, the Reedereigemeinschaft Forschungsschiffahrt GmbH, located in Bremen, Germany. The latter is responsible for hiring, provisioning, and coordinating ship maintenance. Used for ocean research primarily in the Atlantic and Indian Oceans, the R/V *Meteor* routinely carries scientists from many different countries. Construction

of the Meteor was completed in 1986 in Travemunde, Germany. The basic features of the vessel are as follows:

Port of registration	Hamburg				
Call sign	DBBH				
Classification	GL+100A4E2+MC Auto				
Operator	Institut für Meereskunde, Universität Hamburg				
Built	1985–1986 at Schlichting Werft, Travemunde, West Germany				
<b>Basic dimensions:</b>					
Gross registered tonnage	3990				
Net registered tonnage	1284				
Displacement	4780 t				
Overall length	97.50 m				
Beam	16.50 m				
Draught max.	5.60 m				
Service speed	12 kn				
Depth main deck	7.70 m				
Personnel	Crew: 32; scientists: 30				
Main engine	$4 \times Mak6M 322 = 4 \times 1000 \text{ kW}$ at 750 rpm				
Propulsion	Diesel-electrical, tandem-motor = $2 \times 1150$ kW				
Fuel consumption	~12.0 t IFO-80 per day at service speed				
Maximum cruise duration	60 days				
Nautical equipment	Integrated navigation system with data transfer to position computer, echosounder synchronization and supervision, and				
<b>a</b> •	data-processing facility				
Science quarters	20 laboratories on the main deck with ~400 m <sup>2</sup> of working				

space for multidisciplinary research

R/V Meteor (I) was constructed in 1925, the first research and survey vessel of that name. Owned by the German navy, it was based in Wilhelmshaven. One of its first expeditions was the German Atlantic Ocean Expedition of 1925-27, which was organized by the Institute of Marine Research in Berlin. Thereafter, the vessel was used for German physical, chemical, and microbiological marine investigations and for German navy surveying and fisheries protection duties.

R/V Meteor (II) was planned after the 1950s; it was operated by the Deutsche Forschungsgemeinschaft (German Science Community) in Bad Godesberg and by the Deutsches Hydrographisches Institut (German Hydrographic Institute) in Hamburg. Commissioned in 1964, R/V Meteor (II) participated in the International Indian Ocean Expedition.

Multipurpose R/V Meteor (III), used on the cruise described in this documentation, was completed in 1986 and replaced R/V Meteor (II). Based in Hamburg, it is used for German ocean research worldwide and for cooperative efforts with other nations researching in this field. The vessel serves scientists of all marine disciplines in all of the world's oceans.

## **2.2 Cruise Information**

Information about the R/V Meteor 18/1 cruise is summarized as follows:

Ship name	Meteor
Cruise/leg	18/1
Ports of call	Reykjavik, Iceland to Hamburg, Germany
Dates	September 2-25, 1991
<b>Funding support</b>	German Science Community;
	Federal Ministry of Research and Technology, Bonn, Germany; and U.S. Department of Energy (DOE)
Chief Scientist	Professor Dr. Jens Meincke, Institut für Meereskunde, Universität Hamburg, Germany
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#### **Participating Institutions**

BNL	Brookhaven National Laboratory, U.S.A.
BSH	Bundesamt für Seeschiffahrt und Hydrographie, Germany
IFMH	Institut für Meereskunde, Universität Hamburg, Germany
IFMK	Institut für Meereskunde, Universität Kiel, Germany
IUPH	Institut für Umweltphysik, Universität Heidelberg, Germany
SIO	Scripps Institution of Oceanography, U.S.A.
UBP	Universität Bremen, Fachbereich Physik, Germany

### **2.3 Cruise Summary**

The BNL  $CO_2$  group, consisting of K. M. Johnson and R. Ramirez, arrived in Reykjavik, Iceland, on August 29 and went aboard the next day to join the IFMK  $CO_2$  group members, Drs. Bernd Schneider and Lutger Mintrop. Dr. Jens Meincke was already aboard as Chief Scientist. Setting up of the equipment began on August 30 and was completed on the morning of September 2. The R/V *Meteor* departed Reykjavik at 11 a.m. on September 2, 1991. The ship immediately encountered rough weather conditions with gale force winds. Two test stations were completed during the transit across the Denmark Strait to the first station (no. 558) on the South-East Greenland shelf, which was reached on September 5. The earlier gale force winds were replaced by a quiet period characterized by humid air masses over cold water, which resulted in fog. The hydrocast routine was interrupted by winch and rosette bottle-release problems on September 6 and 7 and by currentmeter deployments on September 9, 10, 11, 14, and 19. Bad weather forced several delays on September 13, when the pressure dropped to 980 hPa, wind gusted to 11 Beaufort, and waves rose to 8 m. This scenario was repeated on September 17, and the slowly receding sea conditions thereafter continued to plague the oceanographic work until the end of the hydrographic program of WOCE section A1E at station 622 on September 21. Each rough period was followed by reduced sampling on stations (12 bottles instead of 24 on each rosette), but these stations were restricted to short lines perpendicular to the WOCE line. The station locations are shown in Fig. 1. Of the six stations (592, 593, 595, 606, 607, and 608) taken normal to the WOCE line, only station 607 was sampled for carbonate system parameters. XBT measurements were made at selected CTD stations in parallel with the CTD casts, and acoustic Doppler current profiles (ADCP) were made continuously from September 2 to September 22 to measure the instantaneous near-surface currents.

Two single-operator multiparameter metabolic analyzers (SOMMAs) from BNL (hereafter the systems are designated BNL I and BNL II), one potentiometric alkalinity titrator from IFMK and one ifrared-based system for underway  $pCO_2$  measurements from IFMK, were on board for this cruise. A total of 583 TCO<sub>2</sub> samples, normally collected in conjunction with tracer samples, were taken from 31 section stations, 1 test station (no. 557) and two calibration stations (nos. 581, 608) from a total of 59 bottle casts. Not all 59 stations could be sampled for tracers and TCO<sub>2</sub> because of the limited time available for analysis. The standard WOCE parameters (oxygen, nutrients, and salinity) were sampled on all stations, and on approximately every other station these were augmented by the tracer samples for CFCs, carbonate, helium, tritium, and radiocarbon as the ship steamed eastward from the southeastern tip of Greenland to the coast of Ireland. The density of the CO<sub>2</sub> sampling was fairly constant, ~2 stations per day; the underway pCO<sub>2</sub> system operated continuously.

Both electrical and mechanical problems were noted for each of the SOMMA coulometer systems. BNL II was most severely affected and was declared nonoperational on September 16, when the magnetic valves on the SOMMA chassis could no longer be operated reliably, the electronic calibration factor suddenly changed by +0.11% (a factor of 10 higher than the usual precision of  $\pm 0.01\%$ ), and the communication between the keyboard and PC became erratic. The final Certified Reference Material (CRM) run on this date was 6 µmol/kg lower than the certified value, and test sample duplication was equally poor. When this system was operated several months later in the laboratory, all components functioned satisfactorily, and it was impossible to determine the cause of the shipboard difficulties. BNL I experienced two serious problems. First, the BNL I coulometer became inoperable when the photodetector amplifier failed on September 7. Fortunately, a backup coulometer from Kiel was available, and it was immediately placed in service. Second, the gas calibration system apparently failed on September 10 as a result of cross-talk between the gas sample loops (CO<sub>2</sub> leaking from one loop into the other through a surface scratch or scoring of the valve, which contaminates the carrier gas). This manifested itself as a very noisy system with a very high and unusable blank. The problem was corrected by disconnecting the gas sample valve from the system so that the carrier gas  $(N_2)$  passed directly from the gas cylinder into the SOMMA stripper.

Because of the rough weather, plans for a return voyage around the north of Scotland to Hamburg were changed, and the ship arrived in Hamburg on September 25, via the English Channel, where winds astern arising from a low pressure system near the Faeroe Islands hastened the return voyage.

## **3. DESCRIPTION OF VARIABLES AND METHODS**

The data file **met18.dat** (see descriptions of data files in Part 2) in this numeric data package (NDP) contains the following variables: station numbers; cast numbers; sample numbers; bottle numbers; CTD pressures, temperatures, and salinities; reversing thermometer readings; potential temperatures; bottle salinities; concentrations of dissolved oxygen, silicate, nitrate, nitrite, and phosphate; TCO<sub>2</sub> and TALK concentrations; and quality flags. The station inventory file **m18sta.inv** contains expedition codes, section numbers, station numbers, cast numbers, sampling dates (i.e., month, day, year), sampling times, latitude, longitude, and bottom depth for each station. The data file **uwpco2.dat** contains sampling dates (i.e., day, month, year), sampling times, latitude, longitude, sea surface salinity, sea surface temperature, and underway  $pCO_2$  measurements.

Water samples were collected in 24 General Oceanics 10-L Niskin bottles mounted on a Neil Brown Mark III CTD instrument (S/N NB3) provided by IFMK. Data were acquired at a rate of 32 ms/cycle by using Oceansoft Rev. 3.1. Further details are given by Meincke (1993), and additional data concerning postcruise and precruise laboratory calibrations of the CTD temperature, pressure, conductivity, and oxygen sensors may be found in Siedler and Zenk (1992) and Ruhsam (1994). ADCP measurements to a depth of 300 m were made nearly continuously (with some breaks for rough weather and minor computer malfunctions) from September 2 to 22 with a hull-mounted system from RD Instruments (San Diego) that used a pulse frequency of 150 kHz.

The rosette systems used with the CTD on this cruise experienced various mechanical and electrical problems such that tripping failures were not uncommon—especially at stations 596–613. Repeated checks on board and several careful verifications with the complete bottle data sets were carried out, and the current pressures for each sample are considered correct by the responsible personnel. Reversing thermometers, both electronic (SIS, Kiel) and mechanical (Gohla Precision, Kiel), were also read at the completion of each cast. The processing and quality control of CTD and bottle data performed at BSH followed the guidelines published in the WOCE Operations Manual (WHPO 91-1, 1991). Salinity corrections were made by using bottle salinities measured 1-2 days after collection and determined on a Guildline Autosal model 8400A, which was standardized at each station with reference water (batch P112). Because of temporal conductivity sensor shifts, separate corrections were applied for stations 558–566, 567–602, and 603–622. The final salinity data are expected to be accurate to  $\pm 0.002$  on the Practical Salinity Scale (PSS). Bottle oxygen was determined by Winkler titration following the techniques of Carpenter (1965) and Culberson and Will (1991), by using standards and blanks run in seawater. Subsequently, all Winkler results were recalculated and verified by staff of Oceanographic Data Facility at SIO. The concentrations of nitrate, nitrite, phosphate, and silicate dissolved in seawater were determined for samples collected in high-density polyethylene screw-capped bottles by using a Technicon Autoanalyzer according to procedures given in Hager et al. (1972) and Atlas et al. (1971) and by using the spectrophotometric methods of Armstrong et al. (1967) and Bernhardt and Wilhelms (1967). The analyses were completed within 24 h of sampling, including storage at 6°C for no more than 15 h. Preweighed standards were used to prepare the working standards on board ship.

The  $TCO_2$  concentration was determined by using two SOMMAs described and designed by K. M. Johnson and coworkers (Johnson et al. 1985, 1987; Johnson and Wallace 1992). Along with 158 duplicates, 583 individual samples (total analyzed = 741) from 33 stations (Fig. 2) were collected in 300-mL, precombusted (450°C for 24 h) BOD bottles and immediately poisoned with HgCl<sub>2</sub>, according to DOE's Handbook of Methods for the Analysis of the Various Parameters of the Carbon Dioxide System in Sea Water (DOE 1994). Before analysis the BOD bottles were kept



Figure 2. Sampling depths at all hydrographic stations occupied during R/V Meteor Cruise 18/1.

in darkness in a cold room until thermally equilibrated to the analytical temperature. Dr. Andrew Dickson of SIO supplied 61 CRMs (DOE 1994), which were also analyzed (37 on BNL I and 24 on BNL II). The CRMs were from Batch 7 (B7), which was a filtered sterile salt solution (S = 37.12) spiked with Na<sub>2</sub>CO<sub>3</sub>, and analyzed for TCO<sub>2</sub> by vacuum extraction and manometry in the laboratory of C. D. Keeling at SIO. The certified TCO<sub>2</sub> value was 1926.41 ± 0.82 µmol/kg (n = 13).

Seawater introduced from an automated "to deliver" pipette into a stripping chamber was acidified, and the resultant  $CO_2$ , after drying, was coulometrically titrated on a model 5011 UIC coulometer. In the coulometer cell, the hydroxyethylcarbamic acid that formed from the reaction of  $CO_2$  and ethanolamine was titrated coulometrically (electrolytic generation of OH) with photometric end point detection. The product of the time and the current passed through the cell during the titration was related by Faraday's Constant to the number of moles of OH generated and thus to the moles of  $CO_2$  that reacted with ethanolamine to form the acid. When possible (see text below) the SOMMA-coulometer systems were calibrated with pure  $CO_2$  through the use of hardware consisting of an eight-port gas sampling Valve (GSV) with two sample loops connected to a source of pure  $CO_2$  through an isolation valve with the vent side of the GSV plumbed to a barometer. When a gas loop was filled with  $CO_2$ , the mass (moles) of  $CO_2$  at ambient (*T*) and (*P*). The molar volume of  $CO_2$  [*V*( $CO_2$ )] was calculated iteratively from an expression using the instantaneous barometric pressure (*P*), loop temperature (*T*), gas constant (R), and the first virial coefficient B(*T*) for pure  $CO_2$ :

$$V(CO_2) = RT / P[1 + B(T) / V(CO_2)].$$
(1)

The ratio of the calculated mass to the mass determined coulometrically was the gas calibration factor (CALFAC) used to correct the subsequent titrations for small departures from 100% theoretical response (DOE 1994). The volume of the loops was determined gravimetrically with deionized water by the method of Wilke et al. (1993). When possible (see text below) the standard operating procedure was to make gas calibrations daily or for each new titration cell used (normally one cell per day).

Before the cruise, the "to deliver" volume (TDV) of the SOMMA sample pipette was determined (calibrated) gravimetrically at 20°C with milli-Q deionized water, which had been degassed with Helium. The thermostatted sample pipette was filled with water at the same temperature, and then discharged into preweighed 50-mL serum bottles which were reweighed on a model R300S (Sartorius, Göttingen, Germany) balance. The apparent weight (g) of water collected ( $W_{air}$ ) was corrected to the mass in vacuo ( $M_{vac}$ ) from the following equation:

$$M_{\rm vac} = W_{\rm air} + W_{\rm air}(0.0012/d - 0.0012/8.0) , \qquad (2)$$

where 0.0012 is the sea level density of air at 1 atm, d is the density of the calibration fluid at the pipette temperature and sample salinity, and 8.0 is the density of the stainless steel weights. TDV was calculated by using the following equation:

$$TDV = M_{vac}/d . (3)$$

This procedure was repeated at sea, except the serum bottles were crimp-sealed and reweighed on shore within 3 weeks of collection. The precruise TDV of the pipette for system

BNL I was 28.7108 mL at 20°C. During the cruise the pipette temperature was kept at ~10.2°C  $\pm$  0.3°C. The calculated TDV at 10.2°C (TDV<sub>T2</sub>) was 28.7080 mL:

$$TDV_{T2} = TDV_{T1} [1 + a_v (T_2 - T_1)], \qquad (4)$$

where  $a_v$  is the coefficient of volumetric expansion for pyrex-type glass  $(1 \times 10^{-5} \text{C}^{-1})$ ,  $T_2$  is the measurement temperature, and  $T_1$  is the calibration temperature. The corresponding results for the BNL II pipette were 29.6954 and 29.6925 mL, respectively. During the cruise, eight TDV samples were collected at 10.2°C from the BNL I pipette and sealed for reweighing. The TDV from these weighings was 28.6845 ± 0.0058 mL (0.02%), which differed from the calculated TDV of 28.7080 mL by -0.0235 mL, or -0.082%. For the BNL II pipette, 11 samples were taken at 10.2°C which gave a TDV of the 29.6712 ± 0.0065 mL (0.02%), which differed from the calculated TDV of 29.6925 mL by -0.0213 mL, or -0.072%. Because the original laboratory calibration took place at 20°C, and all of the analytical work aboard ship was done at 10.2°C ± 0.3°C we have used the latter (shipboard) results for TDV to calculate the TCO<sub>2</sub> values (i.e., for BNL I, TDV = 28.6845 mL at 10.2°C; for BNL II, TDV = 29.6712 mL at 10.2°C). These data support the current practice of ensuring identical calibration and analytical temperatures because it appeared that theoretical correction for glass expansion was not adequate to describe the TDV at temperatures significantly different from the calibration temperature (see also DOE 1994).

An IBM-compatible personal computer with two RS232 serial ports, one 24-line digital input/output port, and one analog-to-digital port was used to control the coulometer, barometer, solid state control relays, and temperature sensors, respectively. The temperature sensors (model LM34CH, National Semiconductor, Santa Clara, California), with a voltage output of 10 mV/°F built into the SOMMA, were calibrated against thermistors certified to 0.01°C (PN CSP60BT103M, Thermometrics, Edison, New Jersey) by using a certified mercury thermometer as a secondary standard. These sensors monitored the pipette, gas sample loop, and the coulometer cell temperatures. The barometer, model 216B-101 Digiquartz Transducer (Paroscientific, Inc., Redmond, Washington), was factory-calibrated for pressures between 11.5 and 16.0 psia. The SOMMA software was written in GWBASIC Version 3.20 (Microsoft Corp., Redmond, Washington), and the instrument was driven from the computer.

The analytical method for determination of TCO<sub>2</sub> concentration in seawater used during R/V Meteor Cruise 18/1 differed from the technique described in an earlier data report (Johnson et al. 1995) for R/V Meteor Cruise 15/3 (March 1991). During Cruise 18/1 an electronic calibration procedure was used to check the theoretical response of the coulometers's voltage to frequency converter (VFC) as described in Johnson et al. (1993) and DOE (1994). At least two levels of current (usually 50 and 2 mA) were passed through an independent and very precisely known resistance (R) for a fixed time. The voltage (V) across the resistance was continuously measured, and the instantaneous current (I) across the resistance was calculated from Ohm's law and integrated over the calibration time. Then the number of pulses (counts) accumulated by the VFC during this time was compared with the theoretical number computed from the factory calibration of the VFC [frequency =  $10^5$  pulses (counts) generated per second at 200 mA] and the measured current. If the VFC was perfectly calibrated, electronic calibration yielded a straight line passing through the origin (intercept = 0) with a slope of 1. Calibrations and titrations were done with the coulometer in the counts mode (the total charge passed during a titration was displayed as the number of counts accumulated by the VFC). From the factory calibration of the VFC and the value of the Faraday (96489 Coulomb/mol), a scaling factor of  $4.82445 \times 10^3$ counts/ $\mu$ mol was derived, and the theoretical number micromoles of carbon titrated (M) was determined by the following equation:

#### $M = [\text{counts}/4824.45 - (Blank \times T_{T}) - (INT_{ec} \times I_{T})]/SLOPE_{ec}, \qquad (5)$

where  $T_{\rm T}$  is the length of the titration in minutes, *Blank* is the system blank in µmol/min,  $INT_{ec}$  is the intercept from electronic calibration in µmol/min,  $I_{\rm T}$  the time of continuous current flow in minutes, and  $SLOPE_{ec}$  is the slope from electronic calibration. Note that the slope obtained from the electronic calibration procedure applied for the entire length of the titration, but the intercept applied only for the period of continuous current flow (usually 3–4 min). The TCO<sub>2</sub> concentration in µmol/kg was calculated with the following equation:

$$C_{\rm T} = M \times \text{CALFAC} \times [1/(\text{TDV}_{\rm T} \times \rho)] \times 1.00017 , \qquad (6)$$

where  $C_T$  is the TCO<sub>2</sub>, CALFAC is the gas calibration factor, TDV<sub>T</sub> is the "to deliver" volume of the pipette in mL at the analytical temperature (T),  $\rho$  is the density of seawater in kg/mL from the equation of state (Millero and Poisson 1981), and 1.00017 corrects for the dilution of the sample by the 100 µL of HgCl<sub>2</sub> solution added to the sample bottle.

As a consequence of the coulometer and gas calibration problems described in Sect. 2.3, BNL I was operated between September 13 and September 23 without a gas calibration system. For  $TCO_2$  calculations starting on September 13, the mean CALFAC of 1.002844 (n = 7) obtained for the period September 4–10 was used. No samples were run on BNL I on September 11 and 12. BNL II was continuously operated between September 4 and 15, and calculations were made with the daily gas calibration factors for that instrument. No samples were run on BNL II after September 15. The results of the CRM analyses are shown in Fig. 3 and summaryzed in Table 1.

System	No.	Mean	SD	R. S. D.	Difference		Period
-	(n)	(µmol	/kg)	(%) m	neasured - certif	ïed <sup>a</sup>	(1991)
BNL I <sup>b</sup>	14	1925.87	0.89	0.05	- 0.54	4-10	September
BNL I <sup>c</sup>	23	1925.33	1.46	0.08	- 1.08	13-23	September
BNL II	24	1926.89	1.65	0.09	+ 0.48	4-15	September
Combined	61	1926.07	1.58	0.08	- 0.32	4–23	September

Table 1. Summary of CRM TCO<sub>2</sub> analyses made aboard the R/V *Meteor* during Cruise 18/1 (September 1991) with two SOMMA-Coulometer Systems (BNL I and BNL II).

<sup>a</sup>The CRMs were from Batch 7 and had a salinity of 37.12 and a certified TCO<sub>2</sub> of

 $1926.41 \pm 0.82 \ \mu mol/kg \ (n = 13).$ 

<sup>b</sup>Period with gas calibration unit (September 4–10).

<sup>c</sup> Period without gas calibration unit (September 13–22).

This was the first cruise during which two SOMMA systems were used side-by-side to analyze samples from the same profile and measurements of system precision and bias were made in addition to the CRM analyses. The system precision data are given in Table 2. For these data, "within-sample" precision was the average difference between two replicates analyzed from the same sample bottle, "between-sample" precision was the average difference between duplicate sample bottles taken from the same Niskin bottle, "between-Niskin" precision was the average difference between single sample bottles taken from two Niskin bottles closed at the same depth, and S<sub>p</sub><sup>2</sup> was the pooled standard deviation calculated from multiple "between-sample" replicates Meteor 18; September 1991



Figure 3. Plot of the differences between the measured and certified TCO<sub>2</sub> values for SOMMA - Coulometer Systems I and II during Cruise 18/1 aboard the R/V Meteor. Day # refers to the day of the month during September 1991. (n > 2; stations 557, 581, and 608) analyzed on the same instruments (instrument specific) or from replicates of the same sample analyzed on both instrument (method specific). The  $S_p^2$  was the square root of the pooled variance, according to Youden (1951):

$$S_p^2 = \sqrt{\frac{\sum_{i=1}^{K} \left( \sum_{j=1}^{n_i} (x_{ij} - \bar{x_j})^2 - \left[ \sum_{j=1}^{n_i} (x_{ij} - \bar{x_j}) \right]^2 / n_i \right)}{\sum_{i=1}^{K} n_i - K}}$$

(7)

where K is the number of samples analyzed, and  $\sum_{i=1}^{K} n_i - K$  are the degrees of freedom for the calculation.

Table :	2. Sun	nmary	of sample	preci	sion f	or TCO	O₂ ar	nalyses	made	aboard	the R/V	Meteor
during	Cruise	18/1	September	4-15,	1991	with t	wo S	SOMM.	A-Cou	lometer	Systems	(BNL I
					and	BNL II	0.					

System	M	$S_p^2$		
	Within-sample (n)	Between-sample (n)	Between-Niskin (n)	(K,n)
BNL I	0.77 (18)	0.73 (31)	0.39 (12)	1.49 (3,26) <sup>b</sup>
BNL II	1.10 (19)	0.83 (3)	0.65 (3)	1.68 (2,26) <sup>b</sup>
Cruise totals	0.93 (37)	0.79 (34)	0.52 (15)	1.65 (34,93)°

<sup>a</sup>The mean precision is given as the mean of the absolute differences between duplicates analyzed on the same instrument, i.e.  $\sum_{x=1}^{n} abs (x_1 - x_2)/n$ , where *n* is the number of comparisons between duplicate analyses  $x_1$  and  $x_2$ . See text for explanation of  $S_p^2$ .

<sup>b</sup>Instrument specific.

°Method Specific.

For the instrument specific  $S_p^2$ , K is the number of samples for which more than two replicates were analyzed on the same instrument, and n is the total number of replicates analyzed from K samples. The method specific  $S_p^2$  was calculated from 34 samples (K) for which at least one replicate was analyzed on each instrument [93 replicates (n) analyzed between the two instruments]. If more than one replicate was analyzed on the same instrument, the mean was used to calculate  $S_p^2$  according to the equation from Youden (1951), (Eq. 7). Thus, for the method s pecific calculation  $n_j = K \times 2$  (68 instead of 93). This treatment reduces the degrees of freedom  $(n_j - K)$  to 34 from 59 (93 - K) and yields the most conservative estimate of precision for a single measurement, irrespective of the instrument it was made on. Overall sample precision (method specific  $S_p^2$ ) was  $\pm 1.65 \ \mu mol/kg$  which agreed very well with the precision of the CRM analyses measured on both instruments ( $\pm 1.58 \ \mu mol/kg$ , n = 61, Table 1). Note that BNL I, as a rule, gave slightly better precision than BNL II and that the other precision estimates were consistently better than  $S_p^2$ . However, the higher value of  $\pm 1.65 \ \mu mol/kg$  was considered to be the most conservative estimate of analytical precision because it includes all sources of error—random and systematic—encountered over several days.

System bias was also checked by comparing the calibration station (station 581) samples from a depth of ~2033 m on both instruments over a period of 3-5 days. These data are shown in Table 3. For BNL I, the mean result was  $2159.07 \pm 0.61 \mu mol/kg$  (n = 5, analyzed between September 12 and 16), and the corresponding result for BNL II was  $2158.26 \pm 1.18 \mu mol/kg$  (n = 12, analyzed between September 11 and 13). The absolute value of the difference was 0.81  $\mu mol/kg$  with BNL I giving a slightly higher result. The mean difference and the absolute value of the mean difference between duplicate analyses for the 34 samples used for the calculation of the method specific  $S_p^2$  in Table 2 are shown in Table 3.

Table 3. Summary of TCO <sub>2</sub> analyses for "between sample" duplicates, for which one of
the duplicates was analyzed on SOMMA-Coulometer System BNL I and the other was
analyzed on BNL II aboard the R/V Meteor during Cruise 18/1

Comparison	K	BNL I(n)	BNL II (n)	Difference (I – II)	Abs (I – II)
Station 581 Samples, other	1 34	2159.07 2126.73	2158.26 2128.38	+ 0.81 - 1.65	0.81 1.65
Mean				- 0.42	1.23

Tables 1 and 3 show that BNL I gave slightly lower results in comparison with BNL II for the CRM, and most samples but that was reversed for the test station (581) samples. The sign differences for these data suggests that it would be unwarranted to assign a uniform instrument bias for the duration of the cruise, and accordingly, no correction for instrumental bias has been applied to the data. In effect, it has been decided to accept a conservative estimate of precision that includes an estimate of bias ( $\pm 1.65 \mu mol/kg$ , Table 2) for any single measurement instead of applying a bias correction to the data from either instrument. In aggregate, Tables 1–3 indicate that a single TCO<sub>2</sub> measurement is accurate and precise to  $\pm 1.6 \mu mol/kg$ .

As a final estimate of data quality, duplicate samples from seven Niskin bottles at five stations were collected for later shore-based reference analyses of  $TCO_2$  by vacuum extraction/manometry performed in the laboratory of Dr. Charles Keeling at SIO. The results are given in Table 4, in which the BNL data are compared with the SIO results (Guenther et al. 1994). All samples except the shallow sample from station 580 are clearly consistent with our estimate of accuracy and precision, given previously. Temperature sensors were not included in the shipping crates (as is now standard operating procedure), so the temperature history of these samples between cold storage aboard ship and their arrival at SIO was not known. Table 4 supersedes Tables 3e and 5e from Guenther et al. (1994).

Table 4. Comparison of shipboard analyses of TCO<sub>2</sub> by coulometry (BNL) during the R/V *Meteor* Cruise 18/1 and the shore-based reference analyses of TCO<sub>2</sub> by manometry on duplicate samples in the laboratory of C. D. Keeling at SIO. The reference analyses were made February–March 1994.

Station no.	Sample date	Niskin no.	Depth (m)	TCO <sub>2</sub> (BNL) (µmol/kg)	TCO <sub>2</sub> (SIO) (µmol/kg)	Differ. BNL – SIO	Salinity differ. <sup>a</sup>
575	09.09.91	24	10	2088.25	2087.98	+ 0.27	+ 0.002
575	09.09.91	13	1095	2152.24	2154.55	- 2.31	- 0.019
580	10.09.91	23	27	2085.75	2094.58	- 8.83	- 0.003
580	10.09.91	1	2367	2157.52	2160.00	- 2.48	- 0.003
581 <sup>b</sup>	10.09.91	2	2033	2158.48	2158.73	- 0.25	- 0.004
596	14.09.91	14	690	2167.83	2167.74	+ 0.09	- 0.005
603	16.09.91	1	4063	2202.42	2203.84	- 1.42	- 0.001
Mean o	differences					- 2.13	- 0.005

<sup>a</sup>The difference between the ship's CTD sample salinity and the salinity measured at SIO. <sup>b</sup>Calibration station. The BNL result is the mean of 17 analyses on the two systems between September 11 and 16.

Note that six of the seven differences were within the analytical precision of the methods, and salinities agreed to within 0.005, which rules out evaporative losses.

Total Alkalinity samples were collected in 500-mL bottles with the same precautions as for  $TCO_2$ . Samples were stored in the dark at 4°C and analyzed within 24 h. Samples were transferred into a closed titration cell with a volume of ~120 mL and titrated at 25°C ± 0.1°C with 0.1 *M* HCl containing 0.6 *M* NaCl. The titration cell was based on the systems described by Bradshaw and Brewer (1988) and Millero et al. (1993). The potential was followed with an electrode pair consisting of a ROSS (Orion Inc.) glass pH electrode and a ROSS AgCl reference electrode connected to a high-precision digital voltmeter. The titration was controlled by a computer, which waited for stable emf-readings before adding the next acid increment. The titration curve was analyzed with a modified GRAN-plot method described by Stoll et al. (1993), using the carbonic acid constants of Goyet and Poisson (1989), and taking into account the silicate and phosphate concentrations of the sample to obtain the titration alkalinity. The precision of the method was  $\pm 2.0 \ \mu mol/kg$ , which was determined by replicate analysis of samples. Standardization was accomplished with NaCO<sub>3</sub> standards in NaCl solutions corrected for the blank arising from impurities in the salt.

Underway  $pCO_2$  was measured by using the method of Schneider et al. (1992). Surface seawater was continuously pumped along the cruise track (Fig. 3) at a rate of 200–300 mL/min into a glass equilibrator with a volume of ~300 mL. The seawater was equilibrated with continuously circulating air entering the bottom of the equilibrator through a frit from a closedloop system. This system included a heat exchanger to keep the air at sample temperature, a filter and water trap, and an infrared (IR) analyzer (Siemens, Ultrmat 5F) for the determination of the  $CO_2$  content of the equilibrated air. The infrared analyzer and equilibrator temperature sensor were connected to a computer or to an analog recorder for data display and preservation. The



Figure 4. Track of underway pCO<sub>2</sub> measurements made during R/V Meteor Cruise 18/1.

time constant for the equilibration was ~3 min, which corresponded to a spatial resolution of 0.5 mile with the ship steaming at 10 knots. Atmospheric air was periodically measured, and the system was calibrated every 12 h through the use of calibration gases with  $CO_2$  mixing ratios of 252.5 and 412.8 ppm (v). Pressure corrections were made for the effect of water vapor on total pressure in the equilibrator and the pressure at the inlet of the IR analyzer; the correction for the difference between in situ temperature and measuring temperature was made according to Gordon and Jones (1973). Figure 4 presents the plots of the underway sea surface salinity, temperature, and p $CO_2$  measured during R/V *Meteor* Cruise 18/1.





## 4. DATA CHECKS AND PROCESSING PERFORMED BY CDIAC

An important part of the NDP process at the Carbon Dioxide Information Analysis Center (CDIAC) involves the quality assurance (QA) of data before distribution. Data received at CDIAC are rarely in a condition that would permit immediate distribution, regardless of the source. To guarantee data of the highest possible quality, CDIAC conducts extensive QA reviews that involve examining the data for completeness, reasonableness, and accuracy. Although they have common objectives, these reviews are tailored to each data set, often requiring extensive programming efforts. In short, the QA process is a critical component in the value-added concept of supplying accurate, usable data.

The following summarizes the data processing and QA checks performed by CDIAC on the data obtained during the R/V *Meteor* Cruise 18/1 in the North Atlantic Ocean.

- 1. Carbon-related data and preliminary hydrographic measurements were provided to CDIAC by K. M. Johnson and D. W. R. Wallace of BNL. The final hydrographic and chemical measurements and the station information files were provided by the WOCE Hydrographic Program Office after quality evaluation. A FORTRAN 77 retrieval code was written and used to merge and reformat all data files.
- 2. To check for obvious outliers, all data were plotted using a PLOTNEST.C program written by Stewart C. Sutherland of Lamont-Doherty Earth Observatory. The program plots a series of nested profiles, using the station number as an offset; the first station is defined at the beginning, and subsequent stations are offset by a fixed interval (Figs. 5 and 6).
- 3. To identify "noisy" data and possible systematic, methodological errors, property-property plots for all parameters were generated (Fig. 7) and carefully examined.
- 4. All variables were checked for values that exceeded physical limits, such as sampling depth values exceeding the given bottom depths.
- 5. Dates, times, and coordinates were checked for bogus values (i.e., values of MONTH that were <1 or >12; DAY values <1 or >31; YEAR values ≠1991; TIME values <0000 or >2400; LAT values <49.000 or >65.000; LONG values <-43.000 or >-3.000).
- 6. Station locations (latitudes and longitudes) and sampling times were examined for consistency with maps and with cruise information supplied by K. M. Johnson and D. W. R. Wallace, BNL.
- 7. The designation for missing values, given as -9.0 in the original files, was changed to -999.9.

WOCE Section AlE



Only profiles which exist in this Pressure (dbar) range are plotted. Plotted parameter ranges from 2000 to 2250

Figure 6. Nested profiles: Total carbon (µmol/kg) vs pressure (dbar).

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#### WOCE Section AlE



Only profiles which exist in this Pressure (dbar) range are plotted. Plotted parameter ranges from 2250 to 2450

Figure 7. Nested profiles: Total alkalinity (µmol/kg) vs pressure (dbar).

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## 5. HOW TO OBTAIN THE DATA AND DOCUMENTATION

This database is available on request in machine-readable form, without charge, from CDIAC. CDIAC will also distribute subsets of the database as needed. It can be acquired on 9-track magnetic tape; 8-mm tape; 150-mB, 1/4-in. tape cartridge; IBM-formatted floppy diskettes; or from CDIAC's anonymous File Transfer Protocol (FTP) area through the Internet (see FTP address below). Requests should include any specific media instructions required by the user to access the data (i.e., 1600- or 6250-BPI, labeled or nonlabeled tapes, ASCII or EBCDIC characters, variable- or fixed-length records; 3.5- or 5.25-in. floppy diskettes, high or low density; 8200 or 8500 format, 8-mm tape). Magnetic tape requests not accompanied by specific instructions will be filled on 9-track, 6250-BPI, standard-labeled tapes with EBCDIC characters. Requests should be send to the following address:

Carbon Dioxide Information Analysis Center Oak Ridge National Laboratory Post Office Box 2008 Oak Ridge, Tennessee 37831-6335 U.S.A.

Telephone:(423) 574-0390 or (423) 574-3645Fax:(423) 574-2232

Electronic Mail: cdiac@ornl.gov

The data files can also be acquired from CDIAC's anonymous FTP area through the Internet by following these steps:

• FTP to cdiac.esd.ornl.gov (128.219.24.36),

• Enter "ftp" or "anonymous" as the user ID,

• Enter your electronic mail address as the password (e.g., "alex@alex.esd.ornl.gov")<sup>1</sup>,

• Change to the directory "/pub/ndp056", and

• Acquire the files by using the FTP "get" or "mget" command.

The data files can also be acquired through CDIAC's World Wide Web site at the following address:

http://cdiac.esd.ornl.gov/oceans/home.html

<sup>&</sup>lt;sup>1</sup>Please enter your correct address. This address is used by CDIAC to inform data recipients of data revisions and updates.

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## **PART 2:**

## CONTENT AND FORMAT OF DATA FILES



## 7. FILE DESCRIPTIONS

This section describes the content and format of each of the seven files that compose this NDP (Table 5). Because CDIAC distributes the data set in several ways (e.g., by anonymous FTP, on floppy diskette, on 9-track magnetic tape), each of the five files is referenced by both a file number and an ASCII file name, which is given in lower-case, bold-faced type (e.g., **readme**). The remainder of this section describes or lists the contents of each file. The files are discussed in the order presented in Table 5.

	File number, name, and description	Logical records	File size in bytes	Block size	Record length
1.	readme: A detailed description	1,411	83,319	8,000	80
	of the cruise network, the three FORTRAN 77 data retrieval routines, and the three oceanographic data files				
2.	stainv.for: A FORTRAN 77 data retrieval routine to read and print met18sta.inv (File 5)	36	1,249	8,000	80
3.	met18dat.for: A FORTRAN 77 data retrieval routine to read and print met18.dat (File 6)	44	1,892	8,000	80
4.	uwpco2.for: A FORTRAN 77 data retrieval routine to read and print uwpco2.dat (File 7)	36	1,218	8,000	80
5.	met18sta.inv: A listing of the station locations, sampling dates, and sounding bottom depths for all stations	76	5,598	4,100	41

#### Table 5. Content, size, and format of data files

#### Table 5. (continued)

	File number, name, and description	Logical records	File size in bytes	Block size	Record length
6.	met18.dat:	1,224	192,149	16,000	160
	Hydrographic, carbon dioxide, and nutrient data from all stations				
7.	uwpco2.dat:	2,122	132,833	16,000	120
	Underway pCO <sub>2</sub> data collected along the cruise track				
					• • •
		<u> </u>	<u> </u>		
	Total	4,949	418,258		

## readme (File 1)

This file contains a detailed description of the data set, the three FORTRAN 77 data retrieval routines, and the three oceanographic data files. It exists primarily for the benefit of individuals who acquire this database as machine-readable data files from CDIAC.

#### stainv.for (File 2)

This file contains a FORTRAN 77 data retrieval routine to read and print **met18sta.inv** (File 5). The following is a listing of this program. For additional information regarding variable definitions, variable lengths, variable types, units, and codes, please see the description for **met18sta.inv** on page 33.

5	1 2	<pre>format (2X, 'R/V METEOR CRUISE 18 LEG 1', 5X, 'WOCE LINE A1E', /, 2X, 'EXPOCODE', 2X, 'SECT', 2X, 'STNNBR', 2X, 'CASTNO', 5X, 'DATE', 3X, 'TIME', 5X, 'LATDCM', 5X, 'LONDCM', 3X, 'DEPTH', /)</pre>
6		read (1, 6) format (/////////)
7	1	CONTINUE read (1, 10, end=999) expo, sect, stat, cast, date, time, latdcm, londcm, depth
10	1	format (2X, A8, 3X, A3, 5X, I3, 7X, I1, 3X, A6, 3X, A4, 5X, F6.3, 4X, F7.3, 4X, I4)
	1	write (2, 20) expo, sect, stat, cast, date, time, latdcm, londcm, depth
20	1	format (2X, A8, 3X, A3, 5X, I3, 7X, I1, 3X, A6, 3X, A4, 5X, F6.3, 4X, F7.3, 4X, I4)
999		GOTO 7 close(unit=1) close(unit=2) stop end

#### met18dat.for (File 3)

6

format (/////////////)

This file contains a FORTRAN 77 data retrieval routine to read and print **met18.dat** (File 6). The following is a listing of this program. For additional information regarding variable definitions, variable lengths, variable types, units, and codes, please see the description for **met18.dat** on page 34.

```
**********
c* FORTRAN 77 data retrieval routine to read and print the
                                                                     *
c* file named "met18.dat" (File 6).
CHARACTER bot*3, qualt*10
       INTEGER sta, cast, samp
       REAL pre, ctdtmp, theta, revtmp, ctdsal, salt, oxygen, silcat
       REAL nitrat, nitrit, phspht, tcarb, talk
       OPEN (unit=1, file='met18.dat')
       OPEN (unit=2, file='met18.data')
       write (2, 5)
       format (2X, 'STNNBR', 2X, 'CASTNO', 2X, 'SAMPNO', 2X, 'BTLNBR', 2X,
5
     1 'CTDPRS', 4X, 'CTDTMP', 3X, 'REVTMP', 4X, 'CTDSAL', 5X, 'THETA', 4X
     2 'SALNTY', 2X, 'OXYGEN', 2X, 'SILCAT', 2X, 'NITRAT', 2X, 'NITRIT', 2X,
     3 'PHSPHT', 2X, 'ALKALI', 2X, 'TCARBN', 6X, 'QUALT1', /, 36X, 'DBAR',
4 4X, 'ITS-90', 3X, 'ITS-90', 4X, 'PSS-78', 7X, 'DEG', 4X, 'PSS-78', 1X,
5 7('UMOL/KG', 1X), 10X, '*', /, 25X, '*******', 30X, '*******', 13X,
     6 8('******',1X),10X,'*')
       read (1, 6)
```

31

7 CONTINUE read (1, 10, end=999) sta, cast, samp, bot, pre, ctdtmp, 1 revtmp, ctdsal, theta, salt, oxygen, silcat, nitrat, nitrit, 2 phspht, talk, tcarb, qualt format (5X, I3, 7X, I1, 6X, I2, 5X, A3, 2X, F6.1, 1X, F9.4, 1 1X, F8.3, 1X, F9.4, 1X, F9.4, 1X, F9.4, 2X, F6.1, 1X, F7.2, 2 1X, F7.2, 1X, F7.2, 1X, F7.2, 1X, F7.2, 1X, F7.1, 2X, A10) 10 write (2, 20) sta, cast, samp, bot, pre, ctdtmp, 1 revtmp, ctdsal, theta, salt, oxygen, silcat, nitrat, nitrit, 2 phspht, talk, tcarb, qualt format (5X, I3, 7X, I1, 6X, I2, 5X, A3, 2X, F6.1, 1X, F9.4, 20 1 1X, F8.3, 2X, F9.4, 1X, F9.4, 1X, F9.4, 2X, F6.1, 1X, F7.2, 2 1X, F7.2, 1X, F7.2, 1X, F7.2, 1X, F7.2, 1X, F7.1, 2X, A10) GOTO 7 999 close(unit=1) close(unit=2) stop end

### uwpco2.for (File 4)

This file contains a FORTRAN 77 data retrieval routine to read and print **uwpco2.dat** (File 7). The following is a listing of this program. For additional information regarding variable definitions, variable lengths, variable types, units, and codes, please see the description for **uwpco2.dat** on page 36.

```
c* FORTRAN 77 data retrieval routine to read and print the
c* file named "uwpco2.dat" (File 7)
INTEGER day, month, year
     CHARACTER time*5
     REAL latdcm, londcm, salt, temp, pco2
     OPEN (unit=1, file='uwpco2.dat')
     OPEN (unit=2, file='uwpco2.data')
     write (2, 5)
5
     format (2X,'R/V METEOR CRUISE 18 LEG 1',5X,'WOCE LINE A1E',/,
    1 4X, 'DATE', 6X, 'TIME', 3X, 'LATDCM', 4X, 'LONDCM', 3X, 'SURFSAL',
    2 1X, 'SURFTMP', 2X, 'PCO2', /)
     read (1, 6)
     6
 7
     CONTINUE
     read (1, 10, end=999) day, month, year, time, latdcm,
    1 londcm, salt, temp, pco2
 10
     format (12, 2X, 11, 2X, 14, 2X, A5, 3X, F6.3, 3X, F7.3, 3X,
    1 F7.4, 2X, F5.2, 2X, F5.1)
     write (2, 20) day, month, year, time, latdcm,
```

```
1 londcm, salt, temp, pco2
```

```
20 format (12, 2X, 11, 2X, 14, 2X, A5, 3X, F6.3, 3X, F7.3, 3X,
1 F7.4, 2X, F5.2, 2X, F5.1)
GOTO 7
999 close(unit=1)
close(unit=2)
stop
end
```

## met18sta.inv (File 5)

This file provides station inventory information for each of the 61 stations occupied during the R/V *Meteor* Cruise 18/1. Each line of the file contains an expocode, section number, station number, cast number, sampling date, sampling time, latitude, longitude, and sounding depth. The file is sorted by station number and can be read by using the following FORTRAN 77 code (contained in stainv.for, File 2):

INTEGER stat, cast, depth CHARACTER date\*6, expo\*8, sect\*3, time\*4 REAL latdcm, londcm read (1, 10, end=999) expo, sect, stat, cast, date, time, 1 latdcm, londcm, depth 10 format (2X, A8, 3X, A3, 5X, I3, 7X, I1, 3X, A6, 3X, A4, 5X, 1 F6.3, 4X, F7.3, 4X, I4)

Stated in tabular form, the contents include the following:

Variable	Variable type	Variable width	Starting column	Ending column
expo	Character	8	3	10
sect	Character	3	14	16
stat	Numeric	3	22	24
cast	Numeric	1	32	32
date	Character	6	36	41
time	Character	4	45	48
latdcm	Numeric	6	54	59
londcm	Numeric	7	64	70
depth	Numeric	4	75	78

where

expo

is the expocode of the cruise (i.e., 06MT18/1);

sect	is the WOCE section number (i.e., A1E);
stat	is the station number (values range from 558 to 622);
cast	is the cast number;
date	is the sampling date (month/day/year);
time	is the sampling time (GMT);
latdcm	is the latitude of the station (in decimal degrees; negative values indicate the Southern Hemisphere);
londcm	is the longitude of the station (in decimal degrees; negative values indicate the Western Hemisphere);
depth	is the sounding depth of the station (in meters).

### met18.dat (File 6)

This file provides hydrographic, carbon dioxide, and chemical data for the 61 stations occupied during R/V *Meteor* Cruise 18/1. Each line consists of a station number; cast number; sample number; bottle number; CTD pressure and temperature; potential temperature; reversing thermometer reading; CTD salinity; bottle salinity; concentrations of oxygen, silicate, nitrate, nitrite, phosphate, total carbon dioxide, and total alkalinity; and data quality flags. The file is sorted by station number and pressure and may be read by using the following FORTRAN 77 code (contained in **met18dat.for**, File 3):

```
CHARACTER bot*3, qualt*10
INTEGER sta, cast, samp
REAL pre, ctdtmp, theta, revtmp, ctdsal, salt, oxygen, silcat
REAL nitrat, nitrit, phspht, tcarb, talk
OPEN (unit=1, file='met18.dat')
OPEN (unit=2, file='met18.data')
write (2, 5)
read (1, 10, end=999) sta, cast, samp, bot, pre, ctdtmp,
1 revtmp, ctdsal, theta, salt, oxygen, silcat, nitrat, nitrit,
2 phspht, talk, tcarb, qualt
10 format (5X, I3, 7X, I1, 6X, I2, 5X, A3, 2X, F6.1, 1X, F9.4,
1 1X, F8.3, 2X, F9.4, 1X, F9.4, 1X, F9.4, 2X, F6.1, 1X, F7.2,
2 1X, F7.2, 1X, F7.2, 1X, F7.2, 1X, F7.2, 1X, F7.1, 2X, A10)
```

Stated in tabular form, the contents include the following:

Variable	Variable type	Variable width	Starting column	Ending column
sta	Numeric	3	. 6	8
cast	Numeric	1	16	16
samp	Numeric	2	23	24
bot	Character	3	30	32
pre	Numeric	6.00	35	40
ctdtmp	Numeric	9	42	50
revtmp	Numeric	8	52	59
ctdsal	Numeric	9	61	69
theta	Numeric	9	71	79
salt	Numeric	9	81	89
oxygen	Numeric	6	92	97
silcat	Numeric	7	99	105
nitrat	Numeric	7	107	113
nitrit	Numeric	7	115	121
phspht	Numeric	7	123	129
talk	Numeric	7	131	137
tcarb	Numeric	7	139	145
qualt	Character	10	148	157
where	is the station number;			
cast	is the cast number;			
samp	is the sample number:			an an the second se
ter and the second				
bot <sup>*</sup>	is the bottle number;			
pre de anal	is the CTD pressure (d	bar);		
ctdtmp	is the CTD temperature	e (°C);		
revtmp	is the reversing thermo	meter reading (°C);	e atom a constant. An an atom	n a trib A a trib A a trib
ctdsal*	is the CTD salinity [on	the Practical Salinity	Scale (PSS)];	n a stranger og som en so En som en som e En som en som
theta	is the potential tempera	ature (°C);		
salt <sup>*</sup>	is the bottle salinity:	and a second second Second second		en an trainn an trainn An trainn an

oxygen*	is the oxygen concentration (µmol/kg);			
silcat*	is the silicate concentration (µmol/kg);			
nitrat <sup>*</sup>	is the nitrate concentration (µmol/kg);			
nitrit <sup>*</sup>	is the nitrite concentration (µmol/kg);			
phspht*	is the phosphate concentration (µmol/kg);			
talk*	is the total alkalinity concentration (µmol/kg);			
tcarb*	is the total carbon dioxide concentration (µmol/kg);			
qualt	is a 10-digit character variable that contains data quality parameters flagged by an asterisk (*) in the output file. Quality flag definitions:	flag	codes	for
	<ul> <li>1 = Sample for this measurement was drawn from water bottle not received;</li> </ul>	but a	nalysis	was

- 2 = Acceptable measurement;
- 3 =Questionable measurement;
- 4 = Bad measurement;

5 = Not reported;

- 6 = Mean of replicate measurements;
- 7 = Manual chromatographic peak measurement;
- 8 = Irregular digital chromatographic peak integration;
- 9 = Sample not drawn for this measurement from this bottle.

#### uwpco2.dat (File 7)

This file contains underway  $pCO_2$  measurements taken along the cruise track during the R/V *Meteor* Cruise 18/1. Each line of the file contains a sampling date; sampling time; latitude; longitude; and measurements of sea surface salinity, temperature, and  $pCO_2$ . The file is sorted by date and time and can be read by using the following FORTRAN 77 code (contained in **uwpco2.for**, File 4):

```
INTEGER day, month, year
CHARACTER time*5
REAL latdcm, londcm, salt, temp, pco2
OPEN (unit=1, file='uwpco2.dat')
OPEN (unit=2, file='uwpco2.data')
write (2, 5)
read (1, 10, end=999) day, month, year, time, latdcm,
1 londcm, salt, temp, pco2
format (I2, 2X, I1, 2X, I4, 2X, A5, 3X, F6.3, 3X, F7.3, 3X,
```

10

#### 1 F7.4, 2X, F5.2, 2X, F5.1)

· · ·	· · · · · · · · · · · · · · · · · · ·			· · · · · · · · · · · · · · · · · · ·
Variable	Variable type	Variable width	Starting column	Ending column
dav	Numeric	2	1	2
month	Numeric	1	5	5
year	Numeric	· · · · <b>4</b> · · ·	8	11
time	Character	5	14	18
latdcm	Numeric	6	22	27
londcm	Numeric	7	31	37
salt	Numeric	7	41	47
temp	Numeric	5	50	54
pco2	Numeric	5	57	61
where				
day	is the sampling day;			
month	is the sampling month;			
5 T 3		1		x

Stated in tabular form, the contents include the following:

time is the sampling time (GMT);

year

is the sampling year;

latdcm is the latitude of the station (in decimal degrees; negative values indicate the Southern Hemisphere);

londcm is the longitude of the station (in decimal degrees; negative values indicate the Western Hemisphere);

salt is the sea surface salinity;

temp is the sea surface temperature (°C);

**pco2** is the sea surface  $pCO_2$  (µatm).

## 8. VERIFICATION OF DATA TRANSPORT

The data files contained in this NDP can be read by using the FORTRAN 77 data retrieval programs provided. Users should visually examine each data file to verify that the data were correctly transported to their systems. To facilitate the visual inspection process, partial listings of each data file are provided in Tables 6–8. Each of these tables contains the first and last five lines of a data file.

#### Table 6. Partial listing of "met18sta.inv" (File 5)

First five lines of the file:

06MT18/1	Ale	558	1	090591	1346	60.000	-42.507	185
06MT18/1	Ale	559	1	090591	1607	59.967	-42.175	504
06MT18/1	Ale	560	1	090591	1855	59.930	-41.853	1823
06MT18/1	ALE	561	1	090591	2242	59.895	-41.510	1898
06MT18/1	ALE	562	1	090691	0251	59.863	-41.200	2042
Last five line	s of the f	ile:						
Last five line	s of the f	file:						
Last five line.	s of the f	file:						
Last five line: 06mr18/1	s of the f	file: 618	2	092091	1657	52.335	-15.500	2834
Last five line. 06MT18/1 06MT18/1	s of the f	file: 618 619	2	092091 092091	1657 2251	52.335 52.332	-15.500 -15.218	2834 1262
Last five line: 06MT18/1 06MT18/1 06MT18/1	s of the f AlE AlE AlE AlE	file: 618 619 620	2 1 1	092091 092091 092191	1657 2251 0220	52.335 52.332 52.333	-15.500 -15.218 -14.932	2834 1262 839
Last five line: 06MT18/1 06MT18/1 06MT18/1 06MT18/1	s of the f AlE AlE AlE AlE AlE	file: 618 619 620 621	2 1 1	092091 092091 092191 092191	1657 2251 0220 0508	52.335 52.332 52.333 52.333	-15.500 -15.218 -14.932 -14.643	2834 1262 839 417

Table 7. Partial listing of "met18.dat" (File 6)

First five lines of the file:

558 B44 7,9 6.7531 -999.900 34.7076 6.7524 1 12 34.7090 301.9 2.34 6.54 0.60 -999.90 2086.3 2222244492 0.16 558 6.7531 -999.900 1 13 B42 8.0 34.7065 6.7524 34.7090 301.4 2.54 6.54 0.17 0.57 -999.90 2087.5 2222244492 34.7066 558 11 B46 8.5 6.7571 6.754 6.7563 34.7090 302.4 1 2.34 6.54 0.16 0.60 -999.90 2086.5 2222244492 558 8.7 6.7511 -999.900 34.7059 1 14 K7 6.7503 34.7090 301.6 2.54 6.54 0.16 0.58 -999.90 2087.8 2222244492 558 34.6650 1 10 B45 26.9 6.2526 -999.900 34.6606 6.2503 302.9 2.73 7.23 0.63 2354.00 2091.5 2222244422 0.18

Last five lines of the file:

622 10.0789 -999.900 5 B49 149.2 35.4284 10.0614 35.4340 248.5 5.47 12.21 1 0.00 0.79 -999.90 -999.9 222222299 9.9849 35.4317 622 B43 197.5 9.988 9.9619 35.4560 250.5 4.98 12.11 0.01 0.79 -999.90 -999.9 222222299 622 9.9720 -999.900 35.4517 **K**30 248.0 9.9430 35.4560 251.1 4.98 11.82 3 0.00 0.77 -999.90 -999.9 2222222299 622 296.4 9.8781 9.882 35.4570 9.8436 35.4610 241.3 12.50 2 B46 7.32 1 0.01 0.86 -999.90 -999.9 2222222299 622 1 1 K31 316.0 9.8701 -999.900 35.4589 9.8333 35.4620 239.1 8.01 12.60 0.01 0.87 -999.90 -999.9 222222299

Firs	st fi	ve lines	of the fi	le:	2					
				4 · · · ·						5
3	9	1991	20:20	62.666	-30.026	34.9400	9.13	294.3	•	
3	9	1991	20:25	62.660	-30.057	34.9300	9.30	303.4		
3	9	1991	20:30	62.655	-30.088	34.9267	9.37	307.9		
3	9	1991	20:35	62.648	-30.120	34.9150	9.40	306.6		
3	9	1991	20:40	62.640	-30.151	34.9133	9.40	305.3		
				and the second	- <u>-</u>					
							a			
Las	t fiv	a linas	of the fil	10.						
Lus	ı jır	e unes	oj me ju	к.						
					· · · · · ·			2.		
22	9	1991	19.30	49.722	-4 782	35 3800	15 90	336 1		
22	9	1991	21:00	49.747	-4.353	35.4600	15.70	340.2		
22	9	1991	21:05	49.748	-4.329	35.4800	15.70	340.2		
22	9	1991	21:10	49.750	-4.306	35.4950	15.65	337.2		
22	9	1991	21:15	49.751	-4.282	35.4633	15.70	337.9		
		4			×					
					· 's			1		
				:	1					

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## Table 8. Partial listing of "uwpco2.dat" (File 7)

## **APPENDIX A:**

## STATION INVENTORY



## APPENDIX A: STATION INVENTORY

This appendix lists station inventory information for the 61 sites occupied during the R/V *Meteor* Cruise 18/1 in the North Atlantic Ocean. The meanings of the column headings in Table A-1 are as follows.

is the expocode of the cruise;	
is the WOCE section number;	
is the station number;	
is the cast number;	
is the sampling date (month/day/year);	
	<ul> <li>is the expocode of the cruise;</li> <li>is the WOCE section number;</li> <li>is the station number;</li> <li>is the cast number;</li> <li>is the sampling date (month/day/year);</li> </ul>

**TIME** is the sampling time (GMT);

LATDCM is the latitude of the station (in decimal degrees). Stations in the Southern Hemisphere have negative latitudes;

LONDCM is the longitude of the station (decimal degrees). Stations in the Western Hemisphere have negative longitudes;

**DEPTH** is the sounding bottom depth (in meters).

EXPOCODE	SECT	STNNBR	CASTNO	DATE	TIME	LATDCM	LONDCM	DEPTH
06MT18/1	A1E	558	1	090591	1346	60.000	-42.507	185
06MT18/1	A1E	559	.1	090591	1607	59.967	-42.175	504
06MT18/1	AlE	560	1	090591	1855	59.930	-41.853	1823
06MT18/1	AlE	561	1	090591	2242	59.895	-41.510	1898
06MT18/1	A1E	562	1	090691	0251	59.863	-41.200	2042
06MT18/1	A1E	563	1	090691	0657	59.833	-40.867	2330
06MT18/1	Ale	564	1	090691	1138	59.787	-40.205	2631
06MT18/1	A1E	565	1	090691	1624	59.705	-39.590	2807
06MT18/1	Ale	566	1	090691	2205	59.590	-38.598	3013
06MT18/1	A1E	567	1	090791	1139	59.505	-37.548	3129
06MT18/1	Ale	568	1	090791	1701	59.402	-36.648	3130
06MT18/1	Ale	569	1	090791	2210	59.335	-35.943	3116
06MT18/1	Ale	570	1	090891	0348	59.233	-35.002	2861
06MT18/1	A1E	571	1	090891	1222	59.145	-34.037	2855
06MT18/1	A1E	573	1	090991	0035	59.137	-33.993	2734
06MT18/1	Ale	574	1	090991	0453	59.077	-33.403	2521
06MT18/1	A1E	575	1	090991	0920	59.013	-32.772	2063
06MT18/1	AlE	576	1	090991	1401	58.942	-32.128	1752
06MT18/1	AlE	577	2	090991	2040	58.882	-31.490	1550
06MT18/1	AlE	578	1	091091	0041	58.798	-30.832	1272
06MT18/1	AlE	579	1	091091	0437	58.562	-30.387	1736
06MT18/1	AlE	580	1	091091	0858	58.330	-29.942	2369
06MT18/1	ALE	281	1	091091	1547	58.185	-29.618	2070
06MT18/1	ALE	582	1	091091	1944	58.085	-29.500	2252
06MT18/1	ALE	283	1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1	091191	0020	57.858	-29.057	2333
06Mm19/1	ALC:	204	4	091191	0519	5/.01/	-28.035	2420
06MT18/1	ALC	585		091191	2005	5/.3/0	-20.100	4040
06MT18/1	ALD	500	1	091191	2005	56.914	-27.040	2944
06MT18/1	A1E	588	1	091291	0950	55 992	-27 125	2779
06MT18/1	AIE	589	1	091291	1545	55.533	-26.800	3194
06MT18/1	AlE	590	1	091291	2159	55.068	-26.460	3378
06MT18/1	AlE	591	ī	091391	0505	54.610	-26.118	3420
06MT18/1	A1E	592	1	091491	0256	53.865	-26.285	3643
06MT18/1	A1E	593	1	091491	0656	54.033	-26.018	3319
06MT18/1	A1E	595	1	091491	1407	54.265	-25.600	2554
06MT18/1	Ale	596	1	091491	1741	54.377	-25.950	3229
06MT18/1	A1E	597	1	091491	2254	54.155	-25.762	3156
06MT18/1	A1E	598	1	091591	0334	53.920	-25.637	3622
06MT18/1	Ale	59 <b>9</b>	1	091591	1120	53.672	-25.425	3626
06MT18/1	A1E	600	1	091591	1715	53.463	-24.685	3570
06MT18/1	A1E	601	1	091591	2340	53.267	-23.898	3718
06MT18/1	A1E	602	1	091691	0559	53.068	-23.130	3875
06MT18/1	A1E	603	1	091691	1236	52.858	-22.377	4005
06MT18/1	A1E	604	1	091691	1846	52.655	-21.613	3990
06MT18/1	Aie	605	1	091791	0114	52.467	-20.863	3739
06MT18/1	A1E	607	1	091791	1601	52.497	-20.000	2803
06MT18/1	Ale	608	1	091791	2123	52.175	-19.993	3783
06MT18/1	AlE	609	1	091891	0345	52.358	-20.468	3646
06MT18/1	Ale	610	1	091891	0920	52.337	-20.000	3308
06MT18/1	Ale	611	1	091891	1459	52.337	-19.412	3600
06MT18/1	Ale	612	1	091891	2103	52.323	-18.620	4329
06Wm10/1	ALE	613	1	091991	0402	52.332	-17.815	4292
06Mm10/1	ALE ALE	010	1	091991	1828	52.327	-16.988	3931
0.6Mm10/1	81P	610	4	092091	0119	52.325	-10.202	3465
06MT19/1	312	£10	1	094091	1207	52.338	-15.772	3273
06MT18/1	218	610	2	092091	1657	J4.335 52 325	-15.502	2859
06MT18/1	AIR	£19	1	092091	203/	52 222	-15.300	4034
06MT18/1	AIE	620	1	092191	0220	52 332	-14 932	7202
06MT18/1	AIF	621	1	092191	0508	52.337	-14.643	417
06MT18/1	AIE	622	ī	092191	0737	52.333	-14.253	335
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## Table A.1 Station inventory information for the 61 sites occupied during R/V Meteor Cruise 18/1.

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