

SCOR WG 139:

Organic Ligands- A Key Control on Trace Metal Biogeochemistry in the Ocean

Meeting notes of SCOR WG 139, Meeting 3

Date: 23 February 2014,

Location: Marine Sciences Building, University of Hawaii at Manoa

Present at meeting:

Chairs: Kristen Buck, Maeve Lohan, Sylvia Sander*

Full members: Ron Benner, Kathy Barbeau, Alessandro Tagliabue, Rujun Yang

Associate Members: Constant van den Berg, Thorsten Dittmar, Katsumi Hirose, Phil Boyd, Parthasarathi Chakraborty, Jay Cullen, Christel Hassler

Guests: Christoph Voelker, Bill Landing, David Turner, Eric Achterberg

Apologies: Barbara Sulzenberger, Micha Rijkenberg, Jim Moffett, Peter Croot, Ivanka Pizeta, Mak Saito, Martha Gledhill, Rick Keil, Ken Bruland and François Morel

Agenda

- 8:15 Taxi pick-up from outside the Convention Centre
 - 8:30 Coffee, mingle
 - 9:00 Welcome New Member
 - 9:15 Review of action items from New Orleans Meeting (Buck)
 - 10:00 Intercomparison paper (Sander)
 - 10:30 Coffee
 - 10:50 Recommendations from intercomparison (Sander)
 - 11:30 Field Intercomparison (Lohan)
 - 11:50 Database (Lohan)
 - 12:15 Lunch
 - 13:10 Sensitivity of iron cycle to cycling of organic ligands in a 3D biogeochemical model- Christoph Voelker (20 min plus 20 min discussion)
 - 14:50 How many different ligands exist in seawater- Thorsten Dittmar (20 min plus 20 min discussion)
 - 15:30 Coffee
 - 15:50 Iron and copper binding humic substances in seawater- Stan van den Berg (20 min plus 20 min discussion)
 - 16:30 Overview paper for special issue (Buck)
 - 17:00 Workshop plan (Buck)
 - 17:30 Closing and taxi back to Waikiki
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After a short welcome by Kristen Buck, all people present at the meeting introduced themselves briefly. Kristen went through the last meeting notes and action items.

A review of previous action items

Phil Boyd: Reported on 'omics resources for BATS and Line P. BATS database was found to be easy to use, but no organic data was accessible. For Line P, molecular work coupled with trace metal and speciation studies was conducted during the recent 'GeoMICS' voyage along a portion of Line P, led by Ginger Armbrust, Eric Webb and Jim Moffett (WG member). WG member

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Kathy Barbeau also participated in the cruise. It was noted that an OSM special session on 'omics was planned for Monday. Other collaborative projects mentioned included GEOTRACES and the Tara Oceans and Malaspina Expeditions. This led to a discussion on the importance of coupling biological and organic geochemistry data with trace element measurements, especially in large-scale programs like GEOTRACES. Phil suggested that a letter from this SCOR WG would help strengthen the case for biological and organic data to be collected on GEOTRACES cruises and included in the datasets.

ACTION: Co-chairs will draft a letter to the GEOTRACES SSC on behalf of the WG in support of including biological and organic geochemistry data in the GEOTRACES program.

Maeve Lohan will table the final letter at the October SSC meeting.

Ken Bruland: Summary page of SAFE and BATS metal data, profiles and references submitted by Maeve Lohan.

Kristen Buck: Circulated completed documents to members for editing using Dropbox. Looking for more feedback on the documents.

Added: Re-circulate Dropbox link for document review to members.

All members: **Ongoing:** Review completed documents in Dropbox folder and edit as needed. These will be compiled for the best practices manual and posted on the WG website once complete.

Jay Cullen: Pointed out that the Atlantic might be a better place to target for data compilations of trace elements and speciation given the recent GEOTRACES activities in the basin.

Thorsten Dittmar: **Ongoing:** Provide a summary page with references on organic techniques, target DOM classes for ligands, and related terminology.

Rick Keil: Dropped this action item to move focus to Atlantic data compilations.

Maeve Lohan: Submitted summary pages of SAFE and BATS metal data, profiles and references.

Jim Moffett: Sent summary page for best practices for ACSV measurements. This best practice paper will be combined with Sylvia's summary of references on electrochemistry techniques employed for ligands and information provided by these techniques.

See notes above on Phil's report of 'omics' data and resource of Line P.

Sylvia Sander:

Added: Combine summary pages on electrochemistry techniques, interpretation and references for best practices manual. Post in Dropbox folder for members to review.

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Mak Saito: This information will now be covered in Sylvia's compilation of technique employed. The WG is also already posting new interpretation methods on the website.

Sylvia Sander: Completed the summary page on electrochemistry techniques, and will combine this with Jim's summary for this section of the best practices manual.

All members: **Ongoing**: Provide information to Sylvia for additional links for website.

Maeve Lohan: **Ongoing**: Communicate with Ed Mawji about the proposed parameters for GEOTRACES ligand data submission. Collate data for Zn ligand database.

Kristen Buck: Spoke to Cyndy Chandler at BCO-DMO, including raw speciation data in the database is expected to be fine. Next step is to try an example dataset. Contacted Norm Nelson and Paula Coble about CDOM databases available online, and was provided with links to NASA-CDAS, CLIVAR and a Gulf of Mexico database.

Added: Test a raw speciation dataset on BCO-DMO.

Added: Provide links of CDOM databases to Sylvia for website.

Mak Saito: **Ongoing**: Collate Co speciation data for the database.

Jim Moffett: **Ongoing**: Collate Cu speciation data for the database.

Alessandro Tagliabue: Provided Fe-binding ligand database to chairs.

Added: Send a template to Mak, Jim, and Maeve for the database speciation data compilation, to allow a consistent interface for users.

There was discussion of how to protect the data compiled for the databases, particularly in cases of unpublished data. Sylvia is continuing to look into webpage security.

Thorsten Dittmar: Updated the group on progress with Microsoft program to process DOM results from raw data. This is already partly in use, but has not been officially released.

Sylvia Sander: **Ongoing**: Begin assembling databases on a password-protected page of the WG website. Sylvia reports some IT issues in building the secure site.

Sylvia Sander: Contacted analysts with their letter from the intercalibration exercise. A draft of the manuscript for this exercise has been circulated to participants for review. Discussion of this exercise and manuscript was an agenda item for the meeting, led by Sylvia, see notes below.

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Sylvia Sander and Ivanka Pizeta: **Ongoing**: Post links and manuals to the WG website for the programs used to interpret titration data, to simulate titration data from results, and to calculate free metal ion concentrations.

Mak Saito: Action item to provide a summary of ASV and ACSV interpretation approaches in use, with references and noting labs currently employing them obsolete given the recent release of a program in Excel (KMS) by Bob Hudson for titration interpretation.

ACTION: Sylvia Sander and Ivanka Pizeta provide a link and manual on the WG website for this program.

Maeve Lohan: **Ongoing**: Send an e-mail requesting participants from the e-mail list in the field intercalibration exercises. Discussion of the field intercalibration effort was an agenda item for this meeting, led by Maeve. See notes below.

Kristen Buck: Ed Urban responded to the minutes by suggesting that we talk to GEOTRACES about mediating sample collection costs for the intercalibration, as SCOR does not have funds for this type of activity.

Kathy Barbeau: Noted that there was very limited size-fractionated ligand data at BATS and proposed broadening the target area to include the rest of the North Atlantic. Ron noted that merging size-fractionated ligand and DOM datasets may be complicated by differences in operational definitions of the size fractions.

Ron Benner: **Ongoing**: Provide a list of size-fractionated DOM components to target in future metal ligand studies. Ron noted that he was presenting size-fractionated DOM data in a poster during the OSM (see abstract: <http://www.sgmeet.com/osm2014/viewabstract.asp?AbstractID=14793>).

Kristen Buck: Submitted summary of metal ligand data and references from BATS studies. Assembled published Fe speciation data from Fe fertilization studies, which do not show a consistent response in ligand concentrations upon Fe addition. It was also noted that there is a database of Fe fertilization results available.

ACTION: Phil Boyd will send link for the database to Sylvia to post on the WG website.

Jay Cullen: Compiling metal-ligand data from Line P will be postponed in favor of changing focus to the recent Atlantic GEOTRACES cruises. Ron commented that DOC is relatively invariable with depth below the surface and that it may be more useful to look at targeted compounds of interest, such as lignin.

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Sylvia Sander: Organized a special issue for this WG in Marine Chemistry. This was a separate agenda item for this meeting, led by Kristen, see additional discussion of this topic below.

Christel Hassler: Sent information on CSF conferences as a possible venue for the WG workshop and symposium. Discussion of the final workshop and symposium was an agenda item for this meeting, led by Kristen, see notes below.

Kathy Barbeau: Sent information on OCB scoping workshops as a possible venue for the WG workshop and symposium. Discussion of the final workshop and symposium was an agenda item for this meeting, led by Kristen, see notes below.

Maeve Lohan: Successfully submitted for a special session on metal-binding ligands at the OSM, which included a combination of 8 oral presentations and a poster session (15 posters). Roughly half of the presentations (4 oral, 7 poster) included one or more WG members as co-author.

Intercomparison Paper Discussion

Sylvia gave a presentation updating the group on the intercomparison paper, which is available on the WG website (<http://neon.otago.ac.nz/research/scor/meetings.html>).

Recommendations from Intercomparison Exercise

Recommendations resulting from the intercomparison exercise were outlined with the paper discussion in the same presentation given by Sylvia. A pdf copy of the presentation is posted on the WG website (<http://neon.otago.ac.nz/research/scor/meetings.html>).

Sylvia also noted that the interpretation and simulation programs written by Dario Omanovic and Bob Hudson are freely available, with notes on how to reference the authors, on the WG website (<http://neon.otago.ac.nz/research/scor/achievements.html>).

Field Intercomparison Exercise

Maeve had offered to take samples for a field intercalibration during a Celtic Sea (UK) cruise rescheduled in July 2014 but may have to be rescheduled for 2015. An inquiry to SCOR revealed that SCOR cannot pay for shipment of samples. The general question of: 'do we need the field intercalibration' was raised again, but answered with yes as it is important for quality assurance to have reference values of some samples. The question then was how the logistics and cost of it can be taken care of. Kristen proposes to do similarly to the SAFE intercalibration exercise, i.e. people have to pay for shipment of samples. However, Maeve points out that there is no money or time to provide the acid cleaned bottles in advance. She proposed that participants send their own bottles. Pros and cons of that were discussed. Jay suggested we buy pre-cleaned bottles from a supplier (e.g., SeaStar), but again the lack of funding is prohibitive to this option and concerns regarding the cleanliness of these bottles were also raised. Alessandro commented that

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the intercalibration should include effects from sampling, shipping, bottles, etc. in order to be a realistic intercomparison of everybody's working procedures.

It was decided that Kristen/Maeve will look into how much pre-cleaned bottles cost but that the majority of samples will be collected into bottles people send to Maeve.

ACTION: Kristen Buck: Investigate cost of pre-cleaned bottles for field exercise, with input from Maeve on participation numbers and shipping logistics.

Maeve Lohan: Email the WG email list to determine number of participants in the field intercomparison exercise.

Discussion of Database for Ligands

Database for ligands should be similar to Alessandro's database for iron. Data needs to be safe so people can provide not only published data, but also yet unpublished. BCO-DMO database proposed, but the open accessibility would make this an issue.

The question of which and how data should be in the database, e.g., published vs. unpublished data, results only, or also raw data. Kristen commented that raw data could be unweildly. The database could be flagged if raw data is available.

It was stressed by Maeve that this database for ligands would greatly add to the credibility of SCOR WG 139 group and should be pushed forward. During the OSM Town Hall meeting on Thursday 27 Feb.2014 the attendees will be ask to supply their data. To keep the workload at a realistic level it was agree that data for different metals and their ligands will be collated by the following people:

Jim Moffett: Cu

Maeve Lohan: Zn

Alessandro Tagliabue: Fe

Mak Saito: Co

Invited Talks

Presentations from this meeting will be posted in PDF form on the WG website.

Special Issue in Marine Chemistry

We received expressions of interest for 29 manuscripts to go into the special issue, which is a fantastic number. Below are the most important facts and deadlines for this special issue.

Working title :	SCOR WG 139: Organic Ligands – A Key Control on Trace Metal Biogeochemistry in the
Short Issue Title :	Organic Ligands
Guest Editors:	Sylvia Sander, Kristen Buck and Maeve Lohan
Date first submission expected	01-Feb-2014
Final deadline for submission	31-May-2014

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Final deadline for acceptance	30-Nov-2014
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Online submission is via the Marine Chemistry/ Elsevier web portal. Maeve, Sylvia and Kristen will write an overview article. Other WG members are welcome to contribute to this overview article as well and should contact any of the three co-chairs.

ACTION: Co-chairs will write an overview paper for the special issue, and follow up with contributors on progress toward meeting submission deadline.

Workshop and Symposium in 2015

Christel Hassler, Kathy Barbeau and Ivanka Pizeta informed the co-chairs about options to host the 2015 SCOR WG 139 community-wide workshop and symposium. The offer from Ivanka Pizeta to hold the workshop in Croatia at the Adriatic coast was chosen as a venue, to take place in early April 2015. The program will consist of a one-day training workshop for students, early career scientists and other newcomers to speciation measurements, followed by a two and a half day symposium. The workshop will provide hands-on instruction in CLE-ACSV analyses of seawater samples and data interpretation. The symposium will include updates on WG activities, findings and resources, research talks with discussion, and student/postdoctoral presentations.

Other Business

Phil Boyd mentioned an upcoming Australia-led research cruise with berths available to perform some mesocosm experiments.

Maeve Lohan pointed to the SCOR goals to support and foster collaboration with countries with limited financial abilities. These international research collaborations are fundable by SCOR.

David Turner introduced a new SCOR working group proposal (due mid-April) to develop a web based tool to perform Pitzer speciation modelling for fresh and seawater. Expressions of interest from this WG are welcome and should be directed to David.

At 17.20 pm the SCOR WG 139 Meeting 3 was closed.