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Dataset on optical characteristics and spectroscopic indices of dissolved organic matter of the Kara, Laptev, and East Siberian Seas in August-September 2017

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Article Title

Dataset on optical characteristics and spectroscopic indices of dissolved organic matter of the Kara, Laptev, and East Siberian Seas in August-September 2017.

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Abstract

A total of 137 water samples to study optical properties of chromophoric dissolved organic matter were collected in the Artic shelf seas during the 69th cruise on board the R/V *Akademik Mstislav Keldysh* in August – September 2017. Sampling sites were located in the Kara, Laptev and East Siberian seas and associated to the areas influenced by terrestrial runoff of the Kolyma, Indigirka, Lena, Khatanga, Ob and Yenisei rivers. In this data article, conventional spectroscopic indices and lignin phenol concentrations, calculated on the basis of fluorescence and UV–vis absorption spectra, are presented.

Keywords

Dissolved organic matter, fluorescence, absorbance, spectroscopic indices, Arctic

Specifications Table

Subject	Oceanography
Specific subject area	Optical properties of chromophoric dissolved organic matter
Type of data	Figure Table Text files

How data were acquired	Fluorat-02-Panorama spectrofluorometer (Lumex, Russia) and Solar PB2201 spectrophotometer (Solar, Belarus).
Data format	Raw Analyzed
Parameters for data collection	The sampling depths were chosen based on water mass changes identified with the CTD profiles. Water samples were then collected from Niskin bottles and prepared for further analysis. Fluorescence and absorption spectra were registered at room temperature in the stationary laboratory after the cruise.
Description of data collection	The absorption spectra were measured in a 3-cm or 5-cm quartz-glass cuvette using a dual-beam spectrophotometer against the pure water as a blank. The spectra were measured over the 220-700 nm spectral range in 1 nm increments. The fluorescence spectra were measured in a 1-cm quartz-glass cuvette at excitation wavelengths of 254 nm, 310 nm, and 370 nm.
Data source location	Shelf regions of the Kara, Laptev and East Siberian seas.
Data accessibility	Data on spectroscopic indices and raw spectra are provided with this article.

Value of the Data

- Spectroscopic indices represent efficient tools in tracing dissolved organic matter major sources.
- Data can be used for the water mass characterization and the study of cross-frontal and vertical mixing in the mixing zones of Arctic rivers.
- Under the conditions of climate change, a comparative analysis of the data is of great importance for understanding dynamics of supply and transformation of terrestrial dissolved organic matter in the Arctic basin.

Data

The data presented here come from a complex study of the Arctic shelf seas conducted on board the R/V Akademik Mstislav Keldysh in August-September 2017 [1]. Water sampling to study the cromophoric dissolved organic mater (CDOM) optical properties was performed in the Kara, Laptev, and East Siberian seas at the sites shown in Fig. 1. The studied areas included three cross-shelf sections starting from the estuarine regions of the Khatanga, Indigirka and Kolyma rivers, as well as individual sites in the Kara and Laptev seas. Raw fluorescence and absorption spectra are given in Supplementary materials. Table 1 contains conventional spectroscopic indices, namely humification index *HIX*, index of

recent autochthonous contribution *BIX*, fluorescence index *FI*, spectral slope S_{uvb} , spectral slope ratio S_r and logarithm of lignin phenol concentration calculated on the basis of absorption spectra. The sampling depth and exact sampling date are specified.



Fig. 1. Sampling sites during the 69th cruises of the R/V Akademik Mstislav Keldysh.

Table 1. Spectroscopic indices and lignin phenol concentration of CDOM studied during the 69 th	cruise of
the R/V Akademik Mstislav Keldysh in August-September 2017.	

Station	mon/day/yr	Depth, m	ніх	BIX	FI [9]	FI [10]	S _{uvb} , μm⁻¹	S _r	In(TDLP ₉)
		1	1.6	1	1.5	1.5	23.46	1.77	2.09
	J	10	1.84	1.01	1.27	1.69	23.67	2.07	1.94
5612	09/08/2017	20	2.3	1.01	1.39	1.35	22.87	2.01	1.78
		30	1.52	0.72	1.42	1.55	21.94	2.20	2.08
		47	1.89	0.73	1.57	1.4	21.39	2.04	2.14
	1	3.22	0.87	1.28	1.67	24.13	0.94	2.52	
EC12	00/08/2017	8	2.85	0.87	1.14	1.52	26.11	0.98	2.32
2012	09/08/2017	15	1.72	1	1.13	1.38	24.28	0.91	2.61
		29	2.68	0.95	1.65	1.74	24.22	1.12	1.97
E CA E 00 /00 /00 /00 /00	00/08/2017	1	1.49	0.95	1.47	1.24	26.21	1.39	1.97
2012	09/08/2017	23	2.61	0.77	1.15	1.44	25.84	1.38	2.02
5617 09/09/201		1	3.95	0.82	1.17	1.54	21.33	1.26	3.29
	09/09/2017	13	1.68	0.98	1.47	1.63	25.37	1.28	2.08
		18	1.46	0.85	1.36	1.55	22.12	1.00	2.67
5619	09/09/2017	1	4.96	0.73	1.15	1.4	19.36	1.05	4.05

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		14	5 16	0.82	1 29	1.35	21.81	1.36	3.04
		1	2.85	0.8	1.14	1.55	19.57	1.08	4.09
		6	5.44	0.72	1.21	1.51	18.73	1.08	4.18
5598	09/05/2017	9	6.92	0.8	1.12	1.61	20.97	1.14	3.61
		11	4.52	0.77	1.17	1.63	20.84	1.21	3.57
		0	5	0.81	1.15	1.61	19.36	1.16	4.00
		1	5	0.81	1.15	1.61	19.48	1.21	3.97
5600	09/05/2017	6	4.59	0.81	1.23	1.48	19.49	1.15	3.97
		9	5.43	0.72	1.31	1.59	21.4	1.38	3.35
		17.5	4.87	0.71	1.12	1.55	22.18	1.12	3.31
		1	4.73	0.74	1.15	1.52	20.78	1.06	3.79
		5	n/a	n/a	n/a	n/a	20.91	1.12	3.72
5602	00/06/2017	10	4.24	0.87	1.22	1.58	22.91	1.21	3.22
5002	09/00/2017	16	1.66	0.81	1.36	1.73	23.3	1.24	3.15
		20	5.72	0.69	1.02	1.48	22.39	1.23	3.16
		23	3.46	0.9	1.36	1.52	21.71	1.17	3.28
		1	2.98	0.96	1.26	1.51	22.75	1.25	3.30
	00/06/2017	5	6.42	0.84	1.2	1.39	22.75	1.25	3.23
5604	09/00/2017	11	3.36	0.9	1.41	1.7	23.4	1.24	3.13
		15	3.32	0.98	1.4	1.73	22.32	1.24	3.06
		20.5	2.87	0.93	1.14	1.52	22.68	1.31	2.94
		0	2.93	0.97	1.23	1.33	22.8	1.04	3.00
		1	2.8	0.95	1.23	1.62	23.41	1.07	2.84
EGOE	09/06/2017	10	3.98	0.91	1.17	1.62	22.51	1.04	2.95
5005	03/00/201/	17	2.7	0.91	1.28	1.44	22.65	1.05	2.91
		33	3.64	0.9	1.17	1.69	20.97	1.07	3.16
		41	5.45	0.85	1.15	1.75	21.67	0.99	3.10
		1	4.2	0.89	1.28	1.74	24.45	1.25	2.65
		15	4.78	0.97	1.25	1.36	23.81	1.24	2.76
5606	09/06/2017	25	1.82	0.88	1.35	1.81	23.54	1.18	2.60
		33	3.69	0.86	1.22	1.63	22.84	1.18	2.67
		41	3.43	0.88	1.18	1.70	22.9	1.15	2.70
		0	2.76	0.81	1.30	1.60	21.89	1.00	2.88
		1	4.56	0.91	1.27	1.39	21.8	1.15	3.41
		10	2.73	1.02	1.33	1.55	21.13	1.07	2.82
5607	09/07/2017	20	3.32	0.92	1.14	1.51	20.39	1.12	2.80
		30	3.98	0.88	1.19	1.60	20.79	1.97	3.03
		46	3.49	0.85	1.34	1.65	19.17	1.01	1.99
		54	4.42	0.88	1.26	1.44	20.83	0.92	3.01
5586	08/27/2017	1	1.09	0.98	1.34	1.5	31.37	n/a	1.11
5500	00/2//201/	25	2.21	1.1	1.4	1.65	25.01	n/a	1.42

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				1					
		45	6.84	0.94	1.58	1.71	26	n/a	1.34
		55	1.68	0.94	1.3	1.55	22.79	n/a	1.34
		65	9.62	0.97	1.64	1.5	24.97	n/a	1.33
		75	2.64	0.85	1.37	2.23	24.85	n/a	1.00
		87	9.58	1.07	1.42	1.52	27.41	n/a	0.97
		1	4.84	0.8	1.24	1.51	19.66	1.02	4.04
		5	3.97	0.8	1.17	1.46	19.48	0.98	4.08
		18	3.73	0.91	1.37	1.81	23.4	1.30	3.07
5587	08/28/2017	30	2.47	0.74	1.56	1.76	26.46	1.39	1.53
		60	1.2	0.76	1.33	1.71	25.19	1.80	1.36
		150	2.08	1.09	1.44	1.95	29.32	n/a	0.85
		186	4.05	0.97	1.28	1.84	27.92	n/a	0.80
		1	6.5	0.69	1.21	1.56	17.78	0.98	4.57
		5	6.36	0.75	1.22	1.51	17.82	0.98	4.49
5588	08/28/2017	10	6.49	0.76	1.22	1.48	18.16	1.02	4.19
		20	4.49	0.9	1.2	1.76	20.99	1.17	3.38
		27	4.13	0.84	1.24	1.54	21.2	1.25	2.88
		1	1.05	1.05	1.31	1.51	18.28	n/a	1.15
5612	09/25/2017	10	1.62	0.99	1.74	1.66	17.99	n/a	1.19
5042		50	1.67	1.28	1.47	1.27	16.97	n/a	1.20
		110	3.11	1.03	1.52	1.47	18.63	n/a	0.85
		1	1.86	0.94	1.37	1.4	22.64	1.16	2.46
5641 2	09/26/2017	9	1.48	0.91	1.39	1.88	22.21	n/a	1.64
5041_2	03/20/2017	15	1.78	0.97	1.52	1.52	17.74	n/a	1.44
		76	2.95	0.79	1.22	1.96	16.65	n/a	1.17
		1	2.47	0.99	1.12	1.51	24.84	1.26	2.27
		17	2.63	0.63	1.51	1.31	25.24	1.31	2.26
5590	08/31/2017	30	2.97	0.87	1.26	1.41	23.03	1.21	2.45
5550	00/01/201/	40	3.16	0.82	1.35	1.54	23.64	1.23	2.25
		50	3.37	0.89	1.12	1.88	22.79	1.24	2.32
		62	2.21	0.7	1.18	1.5	22.56	1.18	2.35
		1	5.92	0.64	1.13	1.46	17.08	0.99	4.34
		5	3.6	0.72	1.3	1.49	17.14	1.08	4.16
5591	09/01/2017	10	3.3	0.81	1.11	1.66	20.25	1.39	3.17
0001	,	15	2.84	0.94	1.35	1.68	21.74	1.67	2.68
		30	3.81	0.86	1.1	1.66	21.21	1.53	2.78
		41	5.58	0.69	1.3	1.69	20.5	1.56	2.87
		1	8.63	0.63	1.13	1.49	16.21	0.92	5.19
5627	09/17/2017	5	8.83	0.64	1.14	1.35	16.03	0.94	5.21
		11	6.74	0.66	1.15	1.39	15.81	0.94	5.03
5629	09/17/2017	1	8.1	0.59	1.18	1.51	16.03	0.95	4.96

		12	6.92	0.7	1.16	1.47	15.73	0.99	4.81
		18	6.03	0.59	1.08	1.48	15.83	0.97	4.79
		1	7.68	0.65	1.2	1.39	15.97	0.98	4.67
5620	00/17/2017	14	6.04	0.7	1.14	1.5	15.98	1.00	4.59
5030	09/1//2017	20	5.24	0.63	1.34	1.63	16.08	1.00	4.51
		23	5.38	0.72	1.19	1.61	16.4	1.09	4.13
		1	7.27	0.6	1.14	1.29	16.33	0.95	4.57
5631	09/18/2017	10	7.05	0.68	1.13	1.56	16.4	0.97	4.53
		25	4.71	0.75	1.14	1.43	19.33	1.14	3.22
		1	3.51	0.74	1.18	1.46	17.75	1.10	4.35
5591_2	09/18/2017	13	2.51	0.98	1.2	1.49	n/a	n/a	n/a
		41	2.13	0.84	1.37	1.5	23.25	1.14	2.66
		1	2.94	0.78	1.01	1.39	16.67	1.32	4.21
5633	09/19/2017	18	2.29	0.77	1.43	1.74	22.06	1.67	2.24
		41	2.54	0.8	1.32	1.32	23.25	1.14	2.66
		1	2.54	0.84	1.4	1.59	24.42	1.20	2.59
5590_2	09/19/2017	24	1.69	1.01	1.27	2.15	18.45	2.39	3.89
		59	1.42	0.87	1.39	1.32	24.53	1.28	2.21
		1	1.25	0.88	1.28	1.3	16.08	n/a	3.62
5624	00/10/2017	18	3.61	0.89	1.4	1.5	14.14	2.23	4.03
5054	09/19/2017	80	1.53	1.01	1.18	1.90	n/a	n/a	n/a
		175	n/a	n/a	n/a	n/a	24.79	n/a	0.81
		1	4.73	0.78	1.14	1.49	20.26	1.15	3.64
		10	5	0.81	1.24	1.46	20.35	1.14	3.67
5592	09/02/2017	20	3.77	0.81	1.17	1.52	20.72	1.23	3.02
		32	3.84	0.92	1.4	1.57	23.35	1.53	2.12
		43.5	4.75	0.84	1.34	1.55	22.96	1.63	1.82
	J	1	5.75	0.72	1.26	1.4	18.27	1.09	4.26
		4	6.07	0.7	1.33	1.51	18.09	1.06	4.31
5596	09/03/2017	8	5.92	0.73	1.12	1.46	18.44	1.15	4.12
		17	3.81	0.84	1.33	1.83	20.7	1.32	2.75
		22	3.98	0.91	1.45	1.65	19.69	1.41	2.79
		1	5.33	0.66	1.12	1.51	16.38	0.91	5.26
		5	8.05	0.71	1.17	1.42	16.43	0.98	5.08
5596_2	09/14/2017	8	7.37	0.69	1.17	1.46	n/a	n/a	n/a
		15	3.04	0.8	1.28	1.58	19.82	1.12	3.42
		22.5	2.87	0.77	1.26	1.39	19.53	1.50	3.28
		1	3.95	0.66	1.16	1.55	17.36	1.05	4.65
5592_2	09/14/2017	20	2.69	0.85	1.25	1.57	22.5	1.34	2.97
		44	2.56	0.85	1.21	1.8	16.19	2.08	3.10

n/a – not available

Experimental Design, Materials, and Methods

The sampling depths were chosen based on water mass changes identified with the CTD profiles. Water samples were then collected from Niskin bottles of 5 L volume mounted on the CTD/rosette system. The samples were filtered through precombusted at 450°C Whatman GF/F filters with a pore size of about 0.7 μ m. The filtrate was collected into the acid-cleaned 30 mL glass vials and stored under dark conditions at 4°C until further analysis.

Absorption spectra A_{λ} have been registered at room temperature of 22±2°C with the Solar PB2201 spectrophotometer and 3 or 5 cm quartz cuvettes. The measurements were performed within the spectral range from 220 to 700 nm at 1 nm increments. The blank-corrected absorbance spectra were converted into the Napierian absorption coefficients a_{λ} according to the following equation:

$$a_{\lambda} = \frac{2.303A_{\lambda}}{l} , \qquad (1)$$

where *I* - the cuvette path length in meters.

Absorption spectra within wavelngth ranges 275 - 295 nm and 350 - 400 nm and were characterized by the exponential spectral slope coefficient *S* with respect to the equation suggested by Stedmon et al. [2,3]:

$$a_{\lambda} = a_{\lambda_0} e^{-S(\lambda - \lambda_0)} \tag{2}$$

and depicted as S_{uvb} and S_{uva} , respectively. The values of S_{uvb} and S_{uva} were determined by linear regression of the log-transformed functions of absorption coefficients a_{λ} [4]. The specral slope ratio S_R was calculated as follows

$$S_r = \frac{S_{uvb}}{S_{uva}} .$$
(3)

Dissolved lignin phenol concentrations TDLP₉ were estimated according to the equations reported for the low- and high-CDOM models by Fichot and co-workers [5]:

$\ln(\text{TDLP}_9) = 0.7672a_{350} - 0.3987$	<i>a₂₅₀</i> < 4 m-1;	(4)
$\ln(TDLP_9) = -2.282 \ln(a_{350}) - 8.209 \ln(a_{275}) + 11.265 \ln(a_{295}) + 2.909$	<i>a</i> ₂₅₀ ≥ 4 m-1.	(5)

Fluorescence measurements were performed with a Fluorat-02-Panorama spectrofluorometer (Lumex Instruments) equipped with a Xenon flash lamp as a light source, and a PMT as a detector of luminescence signals. A signal averaging over 20 flashes was applied in order to compensate instability of the flash lamp intensity. The accuracy of excitation and detection wavelength settings was ascertained on a basis of Xe atomic line position and estimated as ±1 nm, spectral resolution of monochromators was 5 nm. Emission scans were acquired at excitation wavelengths λ_{ex} of 254 nm, 310 nm and 370 nm. Fluorescence measurements were performed in 1 cm quartz cuvette. All the spectra were corrected for inner-filter effects. The detected fluorescence intensity at each emission wavelength

was multiplied by $10^{0.5(D_{ex}+D_{em})}$, where D_{ex} and D_{em} represent absorbances at the wavelength of excitation and emission, respectively, related to optical path of 1 cm [6]. Humification index HIX was calculated as a ratio of integral fluorescence intensities

$$HIX = \frac{\sum_{430}^{440} I_{\lambda}}{\sum_{300}^{345} I_{\lambda}}$$
(6)

at excitation wavelength of 254 nm as suggested by Zsolnay et al. [7]. Biological/autochthonous index BIX represent a fluorescence intensity ratio

$$BIX = \frac{I_{380}}{I_{430}} \tag{7}$$

at excitation wavelngth of 310 nm [8]. Two options for the fluorescence index were proposed by McKnight et al. [9] and Cory et al. [10]:

$FI_{\text{McKnight et al.}} = \frac{I_{450}}{I_{500}}$,	(8)
$FI_{\text{Cory et al.}} = \frac{I_{470}}{I_{520}}$.	(9)

In both cases the ratios of fluorescence intensities are considered for the spectra excited at 370 nm.

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