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Supplement of

Spatial and seasonal variability in volatile organic sulfur compounds in seawater and the overlying atmosphere of the Bohai and Yellow seas

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Standard VSC gases with mixing ratios of 1 ppmv were bought from Beijing Minnick Analytical Instrument Equipment Center. Qualitative analysis was conducted by comparing the results with the retention times of the standards, and quantitative analysis was conducted by diluting the VSC standard gases to 1 ppbv and 5 ppbv using a 2202A dynamic dilution meter (Nutech, USA) and injecting different volumes of the diluted VSC standards into the GC using a gas-tight syringe. The VSC mixing ratios were calculated after calibration using standard gases. The VSCs standard curves were obtained as follows: (Fig. S1).
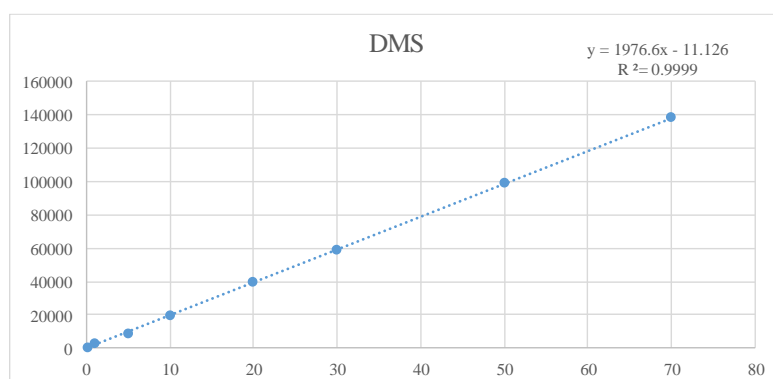
1. VSCs standard curves in spring

(1) COS standard curve:

The 5 ppbv standard gas was used, and the injection volumes were set as 5, 10, 20, 50, 100 mL. We use the standard gas mixing ratio * injection volume (25, 50, 100, 250, 500) as the X-axis, and the peak area detected as Y-axis. The mixing ratios of COS were calculated according to the peak area and correlative equation ($y = 4008.5x + 371580$). The injection volume of atmospheric gas is 200 mL.
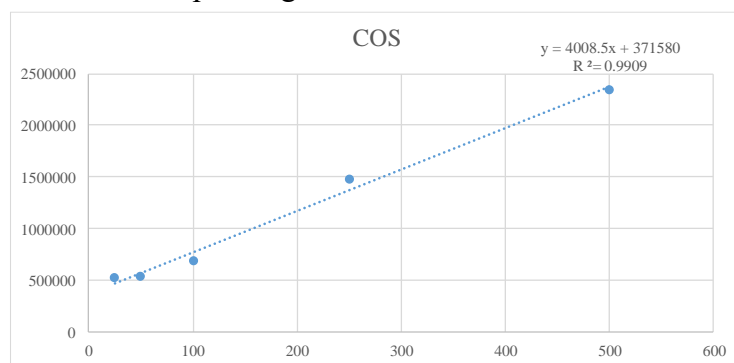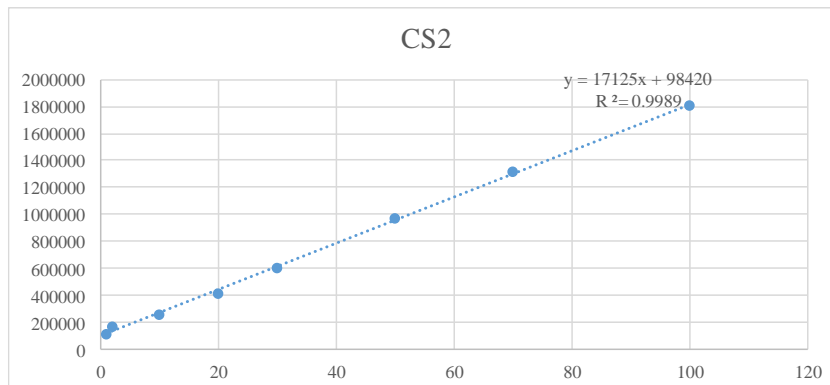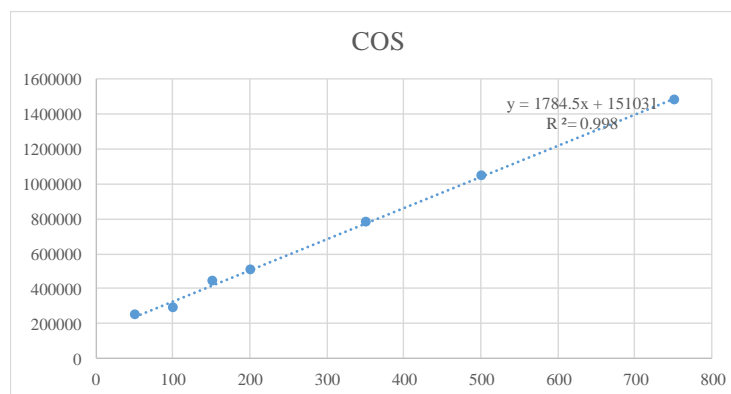

(2) DMS standard curve:

The 1 ppbv standard gas was used, and the injection volumes were set as 0.2, 10, 20, 30, 50, 70 mL. We use the standard gas mixing ratio * injection volume (0.2, 10, 20, 30, 50, 70) as the X-axis, and the peak area detected as Y-axis. The mixing ratios of DMS were calculated according to the peak area and correlative equation ($y = 1976.6\,x - 11.126$).

(3) CS$_2$ standard curve:

The 1 ppbv standard gas was used, and the injection volumes were set as 1, 2, 10, 20, 30, 50, 100 mL. We use the standard gas mixing ratio * injection volume (0.2, 10, 20,

30, 50, 70) as the X-axis, and the peak area detected as Y-axis. The mixing ratios of CS_2 were calculated according to the peak area and correlative equation ($y = 17125x + 98420$).
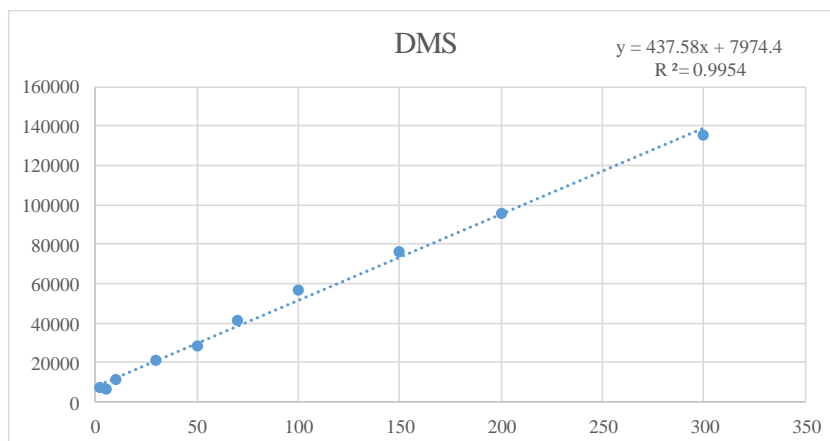

CS2
$y = 17125x + 98420$
$R^2 = 0.9989$

2. VSCs standard curves in summer

(1) COS standard curve:

COS
$y = 1784.5x + 151031$
$R^2 = 0.998$

(2) DMS standard curve:

DMS
$y = 437.58x + 7974.4$
$R^2 = 0.9954$

(3) CS_2 standard curve:

CS2

$y = 3837.7x + 70504$
$R^2 = 0.9942$
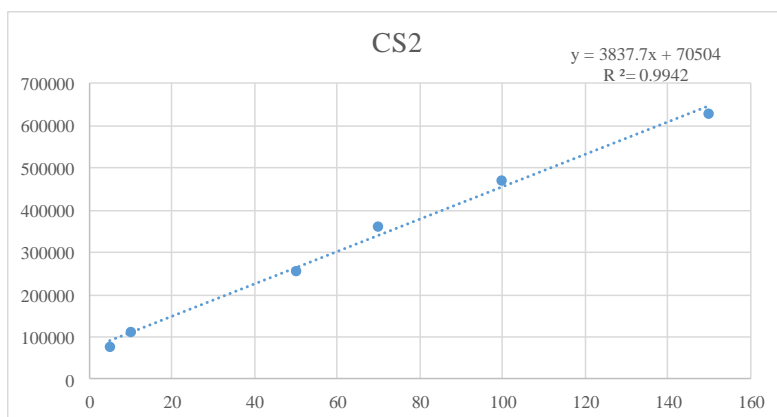
3. The schematics of the instruments were set up as follows:

Pump

He

He

8-way -Valve

GC-MS

First Trap   Second Trap   Third Trap

Canister

Liquid nitrogen
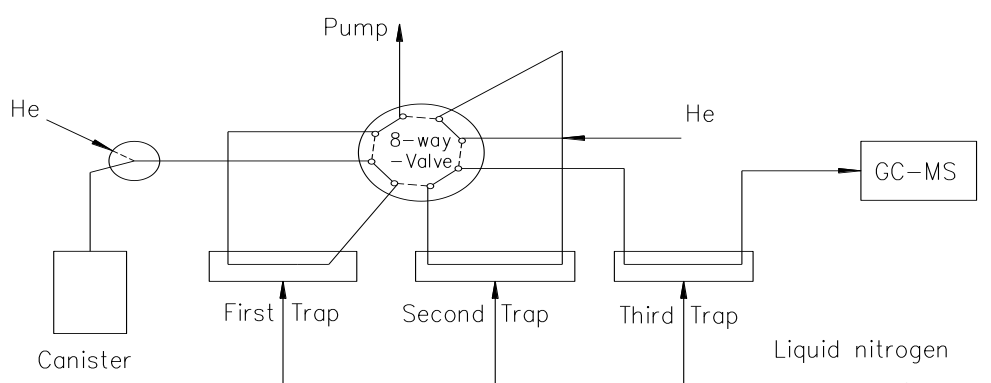
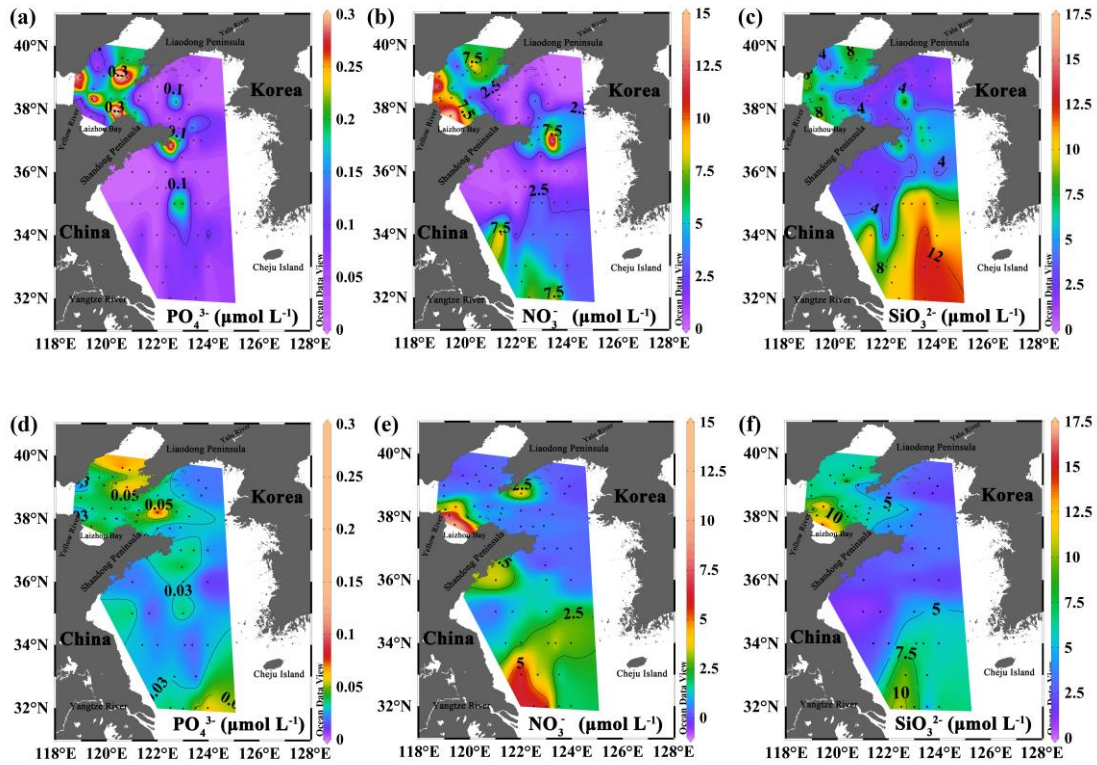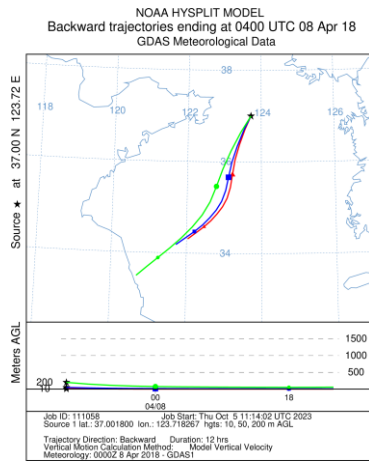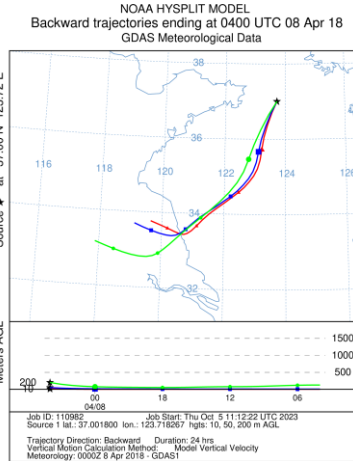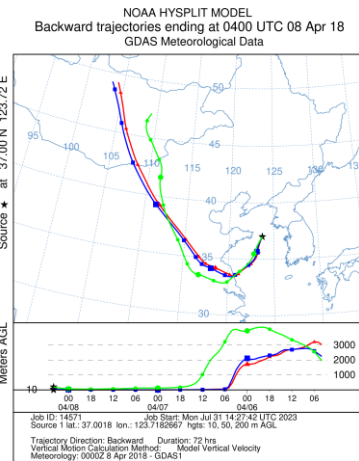Fig. S1 The VSCs standard curves and the apparatus diagram used for analysis of VSCs in atmosphere

Figure S2. Spatial distributions of nitrate, phosphate, and silicate in the surface water of the BS and YS in spring (a)-(c) and summer (d)-(f). The maps were plotted with Ocean Data View (ODV software) (Schlitzer, Reiner, Ocean Data View, odv.awi.de, 2023).
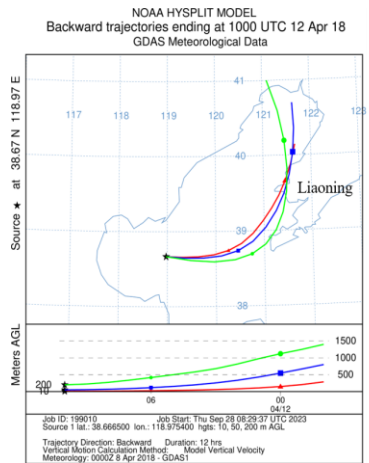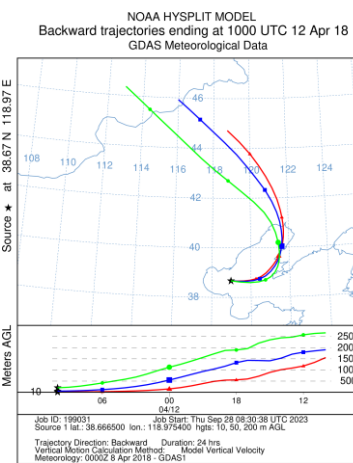
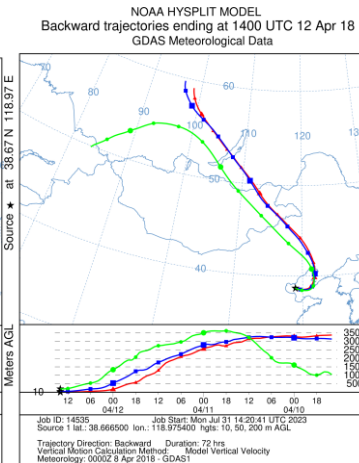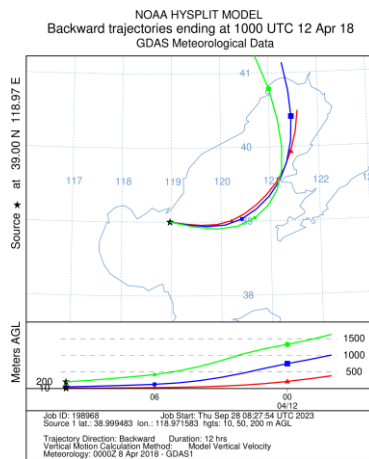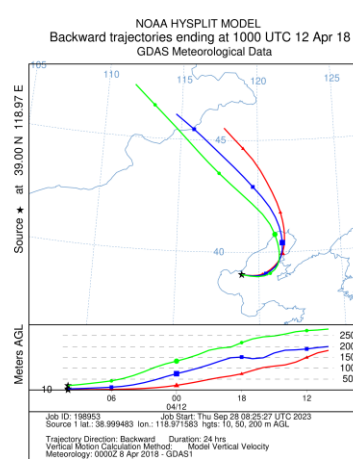B08-spring-12 h   B08- spring-24 h   B08-spring-72 h
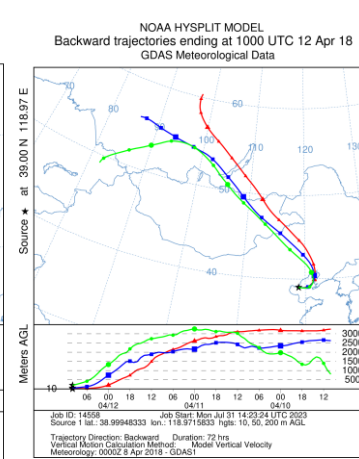
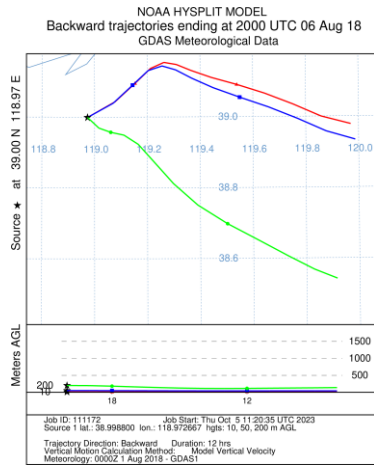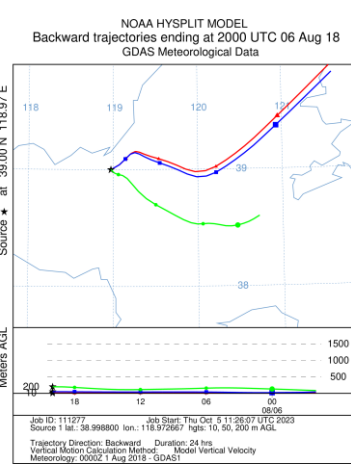B47-spring-12 h   B47- spring-24 h   B47-spring-72 h
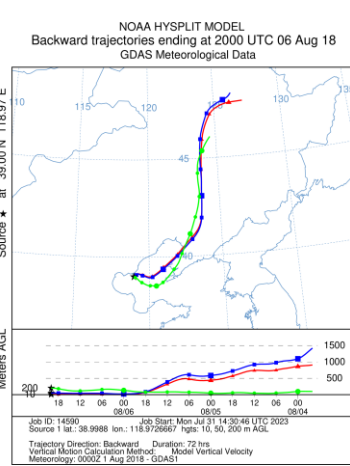
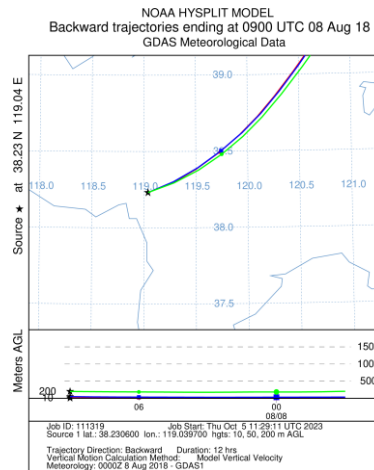B49-spring-12 h   B49- spring-24 h   B49-spring-72 h
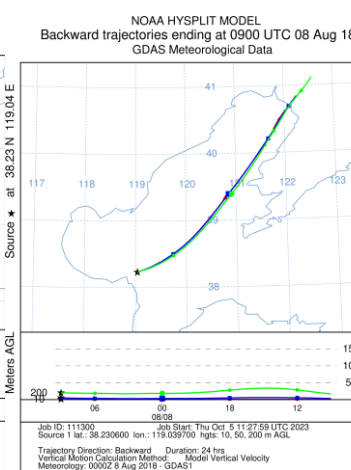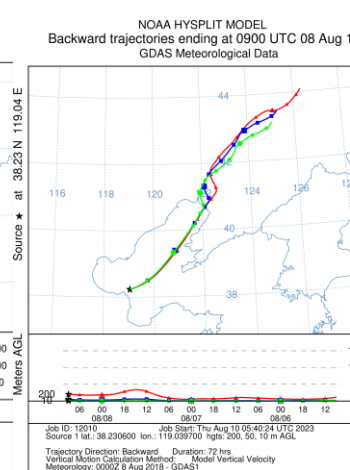
B49-summer-12 h　　　　　B49-summer-24 h　　　　　B49-summer-72 h
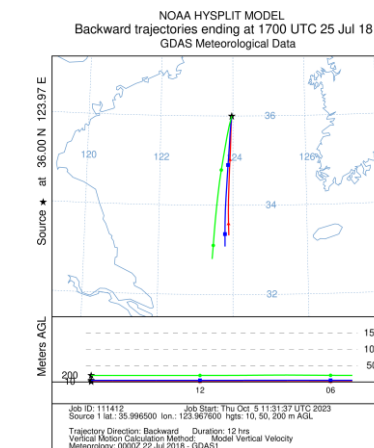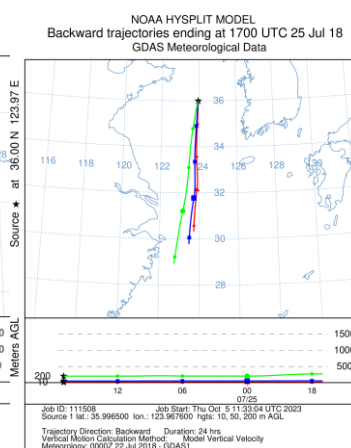

B64-summer-12 h　　　　　B64-summer-24 h　　　　　B64-summer-72 h

H09-summer-12 h　　　　　H09-summer-24 h　　　　　H09-summer-72 h
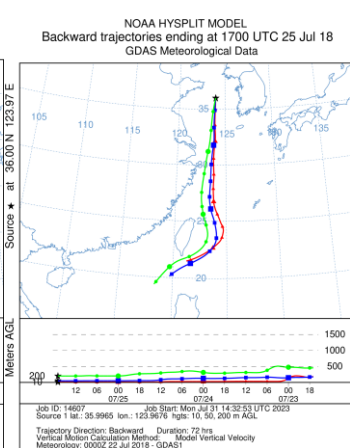
Figure S3. 12 h, 24 h, and 72 h backward trajectories of the air mass above stations

B08, B47, B49 in spring and stations B49, B64, H09 in summer in the BS and YS of

2018.

Table S1. The pre-concentrator parameters of the three-stage cold trap.

Stage	Adsorbent	Trapping temperature T/°C	Preheating temperature T/°C	Stripping temperature T/°C	Baking temperature T/°C	Baking time. t/min
1	Glass beads	-170	20	10	150	2
2	Tenax	-50	-	170	180	2
3	Cryotrapping	-150	-	120	100	2

Table S2. The calculation formulas for Henry's constant. (De Bruyn et al., 1995; Dacey et al., 1984)

	Henry's constant calculation	Parameter
COS	$H = C_1 \mathrm{EXP}[C_2 (1/T - 1/T^{\ominus})]$	$C_1 = 2.2 \times 10^{-2}$ mol L^{-1} atm^{-1}; $C_2 = 2100$K
DMS	$H = C_1 \mathrm{EXP}[C_2 (1/T - 1/T^{\ominus})]$	$C_1 = 5.6 \times 10^{-1}$ mol L^{-1} atm^{-1}; $C_2 = 3500$K
CS$_2$	$H = C_1 \mathrm{EXP}[C_2 (1/T - 1/T^{\ominus})]$	$C_1 = 5.5 \times 10^{-2}$ mol L^{-1} atm^{-1}; $C_2 = 2800$K

The parameterizations for COS, CS$_2$ originate from De Bruyn et al. (1995), and the parameterization for DMS originates from Dacey et al. (1984). $T^{\ominus}$ is standard temperature (298.15 K).

Reference:

Dacey, J. W. H., Wakeham, S. G., and Howes, B. L.: Henry's law constants for dimethylsulfide in freshwater and seawater, Geophys. Res. Lett., 11, 991–994, https://doi.org/10.1029/GL011i010p00991, 1984.

De Bruyn, W. J., Swartz, E., Hu, J. H., Shorter, J. A., Davidovits, P., Worsnop, D. R., Zahniser, M. S., and Kolb, C. E.: Henry's law solubilities and Šetchenow coefficients for biogenic reduced sulfur species obtained from gas-liquid uptake measurements, J. Geophys. Res.-Atmos., 100, 7245–7251, https://doi.org/10.1029/95JD00217, 1995.