Supplementary Information

Carbon Isotope Fractionation during Volatilization of Chlorinated Organic Compounds

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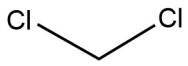
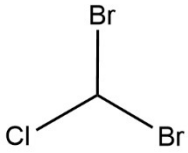
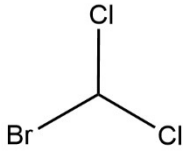
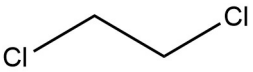
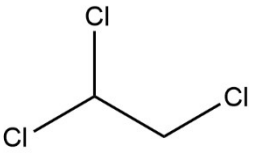
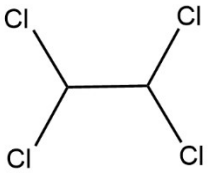
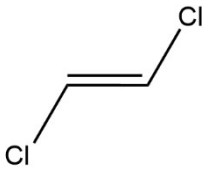
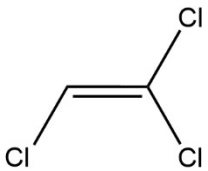
Content:

Table:

Table S1. Properties of the target compounds. Physicochemical data from PubChem.

compound	molecular structure	molar mass (g/mol)	boiling point (°C)	vapour pressure (kPa)
dichloromethane		84.93	40	47.40
chlorodibromomethane		208.28	121	6.09
bromodichloromethane		163.83	90	6.60
1,2-dichloroethane		98.96	83.5	8.70
1,1,2-trichloroethane		133.40	113	2.50
1,1,2,2-tetrachloroethane		167.80	146	0.60
1,2-dichloroethylene		96.94	55	24.00
trichloroethylene		131.38	87	7.80

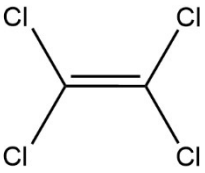
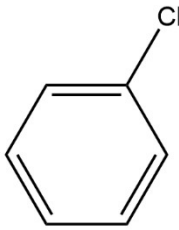
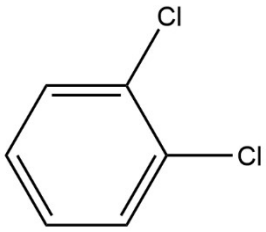
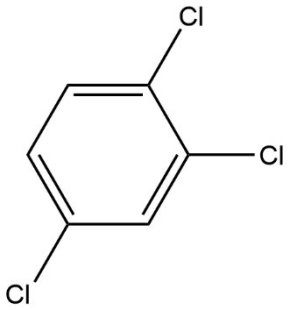
compound	molecular structure	molar mass (g/mol)	boiling point (°C)	vapour pressure (kPa)
tetrachloroethene		165.80	121	1.90
chlorobenzene		112.55	132	1.20
o-dichlorobenzene		147.00	180	0.20
trichlorobenzene		181.40	213	0.03

Table S2. Carbon isotope correlation parameters of chlorinated organic matter during volatilization.

compound	$\delta^{13}C$ (‰)		enrichment factor (‰)
	f = 100%	f = 1%	
dichloromethane	-51.18 ± 0.34	-55.19 ± 0.51	0.10 ± 0.04
chlorodibromomethane	-48.43 ± 0.21	-50.70 ± 0.35	0.61 ± 0.02
bromodichloromethane	-50.00 ± 0.14	-54.60 ± 0.39	1.11 ± 0.05
1,2-dichloroethane	-27.76 ± 0.18	-29.59 ± 0.38	0.40 ± 0.02
1,1,2-trichloroethane	-34.83 ± 0.48	-36.74 ± 0.33	0.44 ± 0.04
1,1,2,2-tetrachloroethane	-19.64 ± 0.54	-22.34 ± 0.17	0.69 ± 0.04
1,2-dichloroethylene	-23.35 ± 0.20	-25.10 ± 0.37	0.41 ± 0.03
trichloroethylene	-23.74 ± 0.25	-26.57 ± 0.53	0.71 ± 0.03
tetrachloroethene	-29.79 ± 0.38	-32.17 ± 0.45	0.57 ± 0.05
chlorobenzene	-25.36 ± 0.23	-27.45 ± 0.28	0.46 ± 0.04

compound	$\delta^{13}C$ (‰)		enrichment factor (‰)
	f = 100%	f = 1%	
o-dichlorobenzene	-24.69 ± 0.37	-26.46 ± 0.35	0.42 ± 0.04
trichlorobenzene	-28.18 ± 0.22	-31.19± 0.33	0.81 ± 0.07

Table S3. Comparison of the $\delta^{13}C$ values of 1,2-dichloroethane, 1,1,2-trichloroethane, tetrachloroethane obtained by GC-IRMS and GC-IRIS (n=4).

compound	GC-IRMS		GC-IRIS	
	$\delta^{13}C$ (‰)	STDV (1σ)	$\delta^{13}C$ (‰)	STDV (1σ)
1,2-dichloroethane	-27.13	0.59	-27.42	0.09
1,1,2-trichloroethane	-34.24	0.41	-34.71	0.41
tetrachloroethane	-20.33	0.21	-20.01	0.21

Carbon CSIA using GC-IRMS. The GC-IRMS includes a Trace 1310 GC (Thermo Scientific, USA) equipped with capillary column (DB-5MS, 30 m×0.25 mm×0.25 μm, Agilent, USA) and split/splitless injector, a GC IsoLink operated at 1030 ℃ and an isotope ratio mass spectrometer (DELTA V Advantage, Thermo Scientific, USA). $^{13}C/^{12}C$ isotopic ratios are reported as $\delta^{13}C$ values by referencing to the VPDB standard (see Eq 1). A software, Isodat, was utilized for data extraction and processing.

Figure:

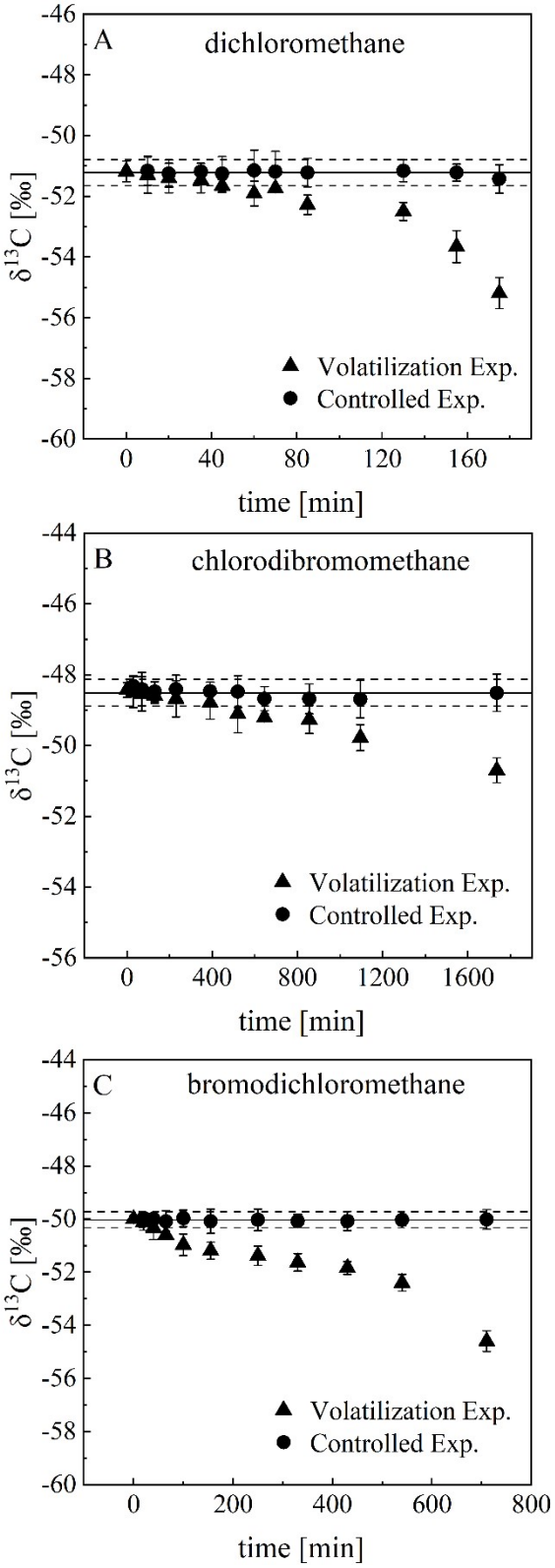


Figure S1. Variations on stable carbon isotope values with time during volatilization of dichloromethane (A), chlorodibromomethane (B) and bromodichloromethane (C).

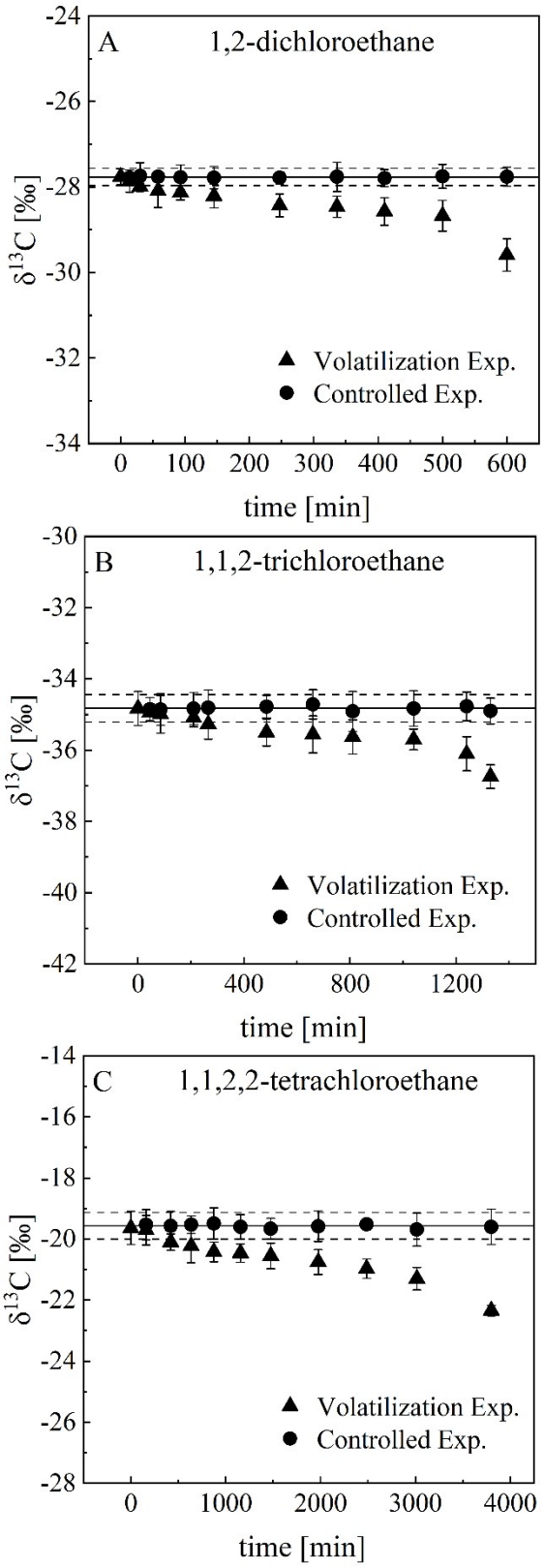


Figure S2. Variations on stable carbon isotope values with time during volatilization of 1,2-dichloroethane (A), 1,1,2-trichloroethane (B) and 1,1,2,2-tetrachloroethane (C).

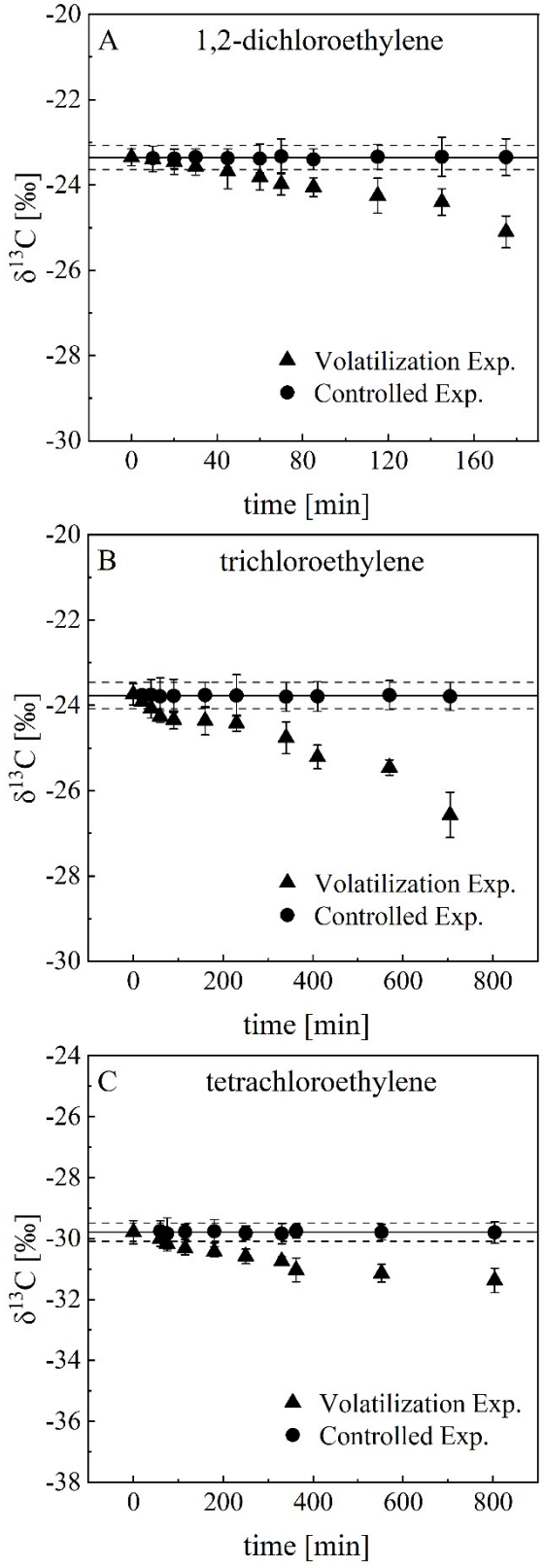


Figure S3. Variations on stable carbon isotope values with time during volatilization of 1,2-dichloroethylene (A), trichloroethylene, (B) and tetrachloroethene (C).

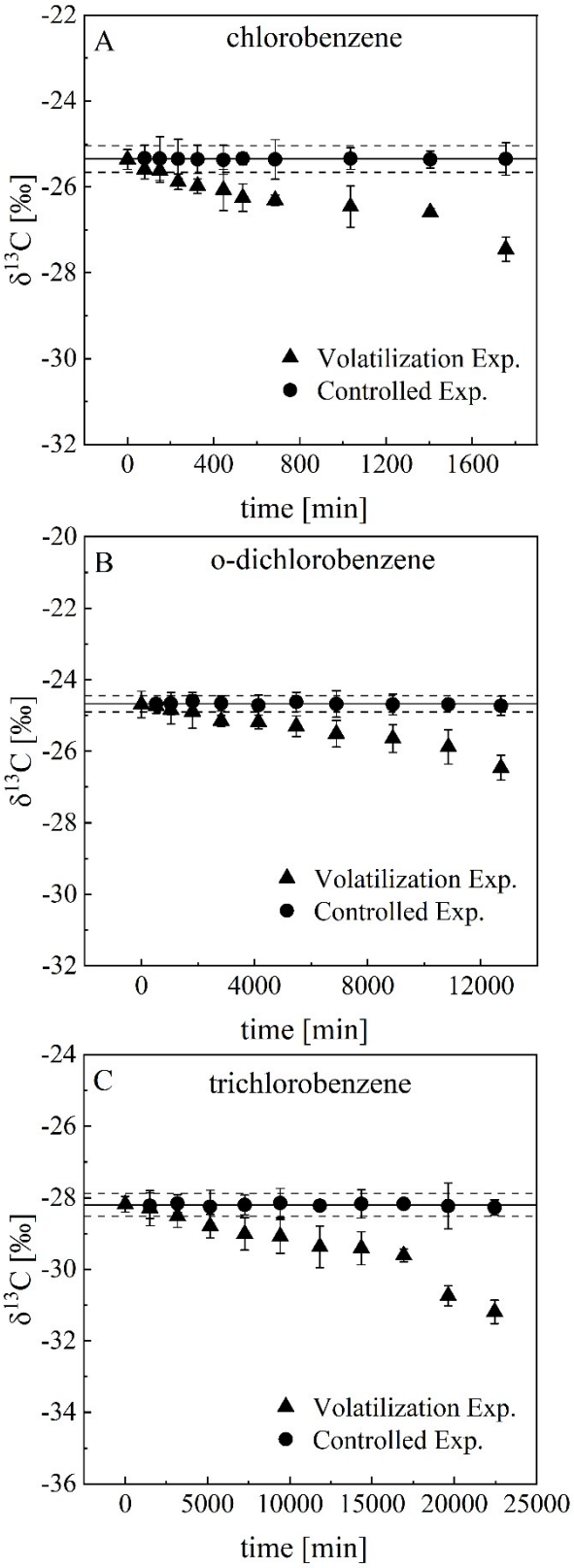


Figure S4. Variations on stable carbon isotope values with time during volatilization of chlorobenzene (A), o-dichlorobenzene (B) and trichlorobenzene (C).