Supporting information

Molecular characterization and source identification of atmospheric particulate organosulfates using ultrahigh resolution mass spectrometry

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This supporting information document contains two tables and two figures.

Table S1: The daily average concentrations of SO_2, NO_2, CO and O_3, average temperature (T) and relative humidity (RH) in Mainz* and Beijing** during the sampling dates.

Sample ID	Sampling Date	SO2 (µg/m3)	NO2 (µg/m3)	CO (mg/m3)	O3 (µg/m3)	T (°C)	RH (%)
MZL	14-01-2015	1	15	0.2	54	5	78
	15-01-2015	1	30	0.27	28	7	73
	16-01-2015	1	32	0.24	36	6	85
BJL	07-01-2014	34	60	2	43	1	22
	08-01-2014	13	21	0.5	53	-2	18
	25-01-2014	24	42	1	61	0	50
BJH	15-01-2014	66	84	2.7	18	-1	62
	22-01-2014	75	93	2.2	16	-1	42
	23-01-2014	118	125	4	8	0	49

* The ambient condition data of Mainz is supported by central immission monitoring network in Rhineland-Palatinate, Germany (www.luft-rlp.de). **The ambient condition data of Beijing is from the open air quality database (www.zq12369.com).

Table S2: Summary of the different isoprene/glyoxyal-, monoterpene-, sesquiterpene-, long-chain alkane-, benzene- and naphthalene-derived OSs and nitrooxy-OSs identified in smog chamber experiments.

Molecular mass	Formula	Precursor	Precursor group
139,97794	C2H4O5S	glycolaldehyde	Isoprene/glyoxyal
143.97286	CH4O6S	glycolaldehyde	
153,99359	C3H6O5S	isoprene	
155,97286	C2H4O6S	glyoxal	
169,98851	C3H6O6S	isoprene	
171.96777	C2H4O7S	glycolaldehyde	
173.98342	C2H6O7S	glycolaldehyde	
187.96269	C2H4O8S	glycolaldehyde	
189.97834	C2H6O8S	glycolaldehyde	
199.96269	C3H4O8S	glycolaldehyde	
199,99907	C4H8O7S	isoprene	
201.97834	C3H6O8S	glycolaldehyde	
211,99907	C5H8O7S	isoprene	
214,01472	C5H10O7S	isoprene	
215.99399	C4H8O8S	glycolaldehyde	
216,03037	C5H12O7S	isoprene	
217.97325	C3H6O9S	glycolaldehyde	
231.98890	C4H8O9S	glycolaldehyde	
245,02054	C5H11NO8S	isoprene	
261,01545	C5H11NO9S	isoprene	
275.97873	C5H8O11S	glycolaldehyde	
302,03077	C8H14O10S	isoprene	

Molecular mass	Formula	Precursor	Precursor group
306,00053	C5H10N2O11S	isoprene	Isoprene/glyoxyal
332,07772	C10H20O10S	isoprene	
334,09337	C10H22O10S	isoprene	
347,01584	C8H13NO12S	isoprene	
452,15636	C15H32O13S	isoprene	
224,03546	C7H12O6S	α-pinene	monoterpenes
227,99399	C5H8O8S	α-pinene	
238,05111	C8H14O6S	α-pinene	
240,03037	C7H12O7S	limonene	
248,07184	C10H16O5S	α-pinene	
250,05111	C9H14O6S	limonene/terpinolene	
250,08749	C10H18O5S	α/β-pinene/terpinolene	
252,06676	C9H16O6S	limonene	
254,04602	C8H14O7S	α-terpinene	
264,06676	C10H16O6S	β-pinene	
266,08241	C10H18O6S	α-pinene/α-terpinene/terpinolene	
268,06167	C9H16O7S	limonene	
280,06167	C10H16O7S	α/β-pinene/terpinolene/lemonene	
282,07732	C10H18O7S	α/β-pinene/limonene/α-terpinene/terpinolene	
284,05659	C9H16O8S	α-terpinene	
284,09297	C10H20O7S	α/β-terpinene/terpinolene	
295,07257	C10H17NO7S	α/β-pinene/α-terpinene/terpinolene	
297,05184	C9H15NO8S	limonene	
298,07224	C10H18O8S	α-pinene/terpinolene	
311,06749	C10H17NO8S	α/β-pinene/α/γ-terpinene/terpinolene	
313,04675	C9H15NO9S	limonene	
327,06240	C10H17NO9S	β-pinene/terpinolene/limonene	
329,07805	C10H19NO9S	limonene	
330,04431	C10H18O8S	α-terpinene	
331,05732	C9H17NO10S	limonene	
340,05765	C10H16N2O9S	α-pinene	
343,05732	C10H17NO10S	α/β-pinene/α-terpinene	
356,05256	C10H16N2O10S	α-pinene	
374,06313	C10H18N2O11S	limonene/terpinolene/α/γ-terpinene	
390,05804	C10H18N2O12S	limonene	
252,06676	C9H16O6S	β-caryophyllene	sesquiterpenes
304,13444	C14H24O5S	β-caryophyllene	
318,15009	C15H26O5S	β-caryophyllene	
320,12936	C14H24O6S	β-caryophyllene	
334,10862	C14H22O7S	β-caryophyllene	
334,14501	C15H26O6S	β-caryophyllene	
348,12427	C15H24O7S	β-caryophyllene	
350,10354	C14H22O8S	β-caryophyllene	
350,13992	C15H26O7S	β-caryophyllene	
352,11919	C14H24O8S	β-caryophyllene	
363,13517	C15H25NO7S	β-caryophyllene	
364,11919	C15H24O8S	β-caryophyllene	
364,15557	C16H28O7S	β-caryophyllene	

Molecular mass	Formula	Precursor	Precursor group
380,15049	C16H28O8S	β-caryophyllene	sesquiterpenes
383,12500	C14H25NO9S	β-caryophyllene	
210,05619	C7H14O5S	dodecane	long-chain alkanes
210,09258	C8H18SO4	octyl OS	
238,08749	C9H18O5S	dodecane	
252,06676	C9H16O6S	β-caryophyllene	
252,10314	C10H20O5S	cyclodecane	
266,08241	C10H18O6S	cyclodecane	
266,15518	C12H26SO4	dodecyl OS	
268,06167	C9H16O7S	decalin	
270,07732	C9H18O7S	decalin	
280,06167	C10H16O7S	cyclodecane	
280,13444	C12H24O5S	dodecane	
286,07224	C9H18O8S	decalin	
296,05659	C10H16O8S	decalin	
298,07224	C10H18O8S	decalin	
304,13444	C14H24O5S	β-caryophyllene	
318,15009	C15H26O5S	β-caryophyllene	
320,12936	C14H24O6S	β-caryophyllene	
327,06240	C10H17NO9S	decalin	
334,10862	C14H22O7S	β-caryophyllene	
334,14501	C15H26O6S	β-caryophyllene	
348,12427	C15H24O7S	β-caryophyllene	
350,10354	C14H22O8S	β-caryophyllene	
350,13992	C15H26O7S	β-caryophyllene	
352,11919	C14H24O8S	β-caryophyllene	
363,13517	C15H25NO7S	β-caryophyllene	
364,11919	C15H24O8S	β-caryophyllene	
364,15557	C16H28O7S	β-caryophyllene	
380,15049	C16H28O8S	β-caryophyllene	
383,12500	C14H25NO9S	β-caryophyllene	
173,99868	C6H6S1O4	benzene	benzene
188,01433	C7H8S1O4	benzene	
202,02998	C8H10S1O4	benzene	
216,04563	C9H12S1O4	benzene	
218,98376	C6H5NO6S	2-methylnaphthalene	naphthalene
232,04054	C9H12O5S	2-methylnaphthalene	
258,01981	C10H10O6S	naphthalene	
274,01472	C10H10O7S	naphthalene	
276,03037	C10H12O7S	naphthalene	
288,03037	C11H12O7S	2-methylnaphthalene	
290,04602	C11H14O7S	2-methylnaphthalene	
321,01545	C10H11NO9S	naphthalene	

Table prepared from the following references: Surratt et al., 2007, 2008, 2010; Lim et al., 2010; Perri et al., 2010; Chan et al., 2011; Riva et al., 2015, 2016; Huang et al., 2018; Wang et al., 2016; Lin et al., 2012; Iinuma et al., 2007, 2009.[1-13]

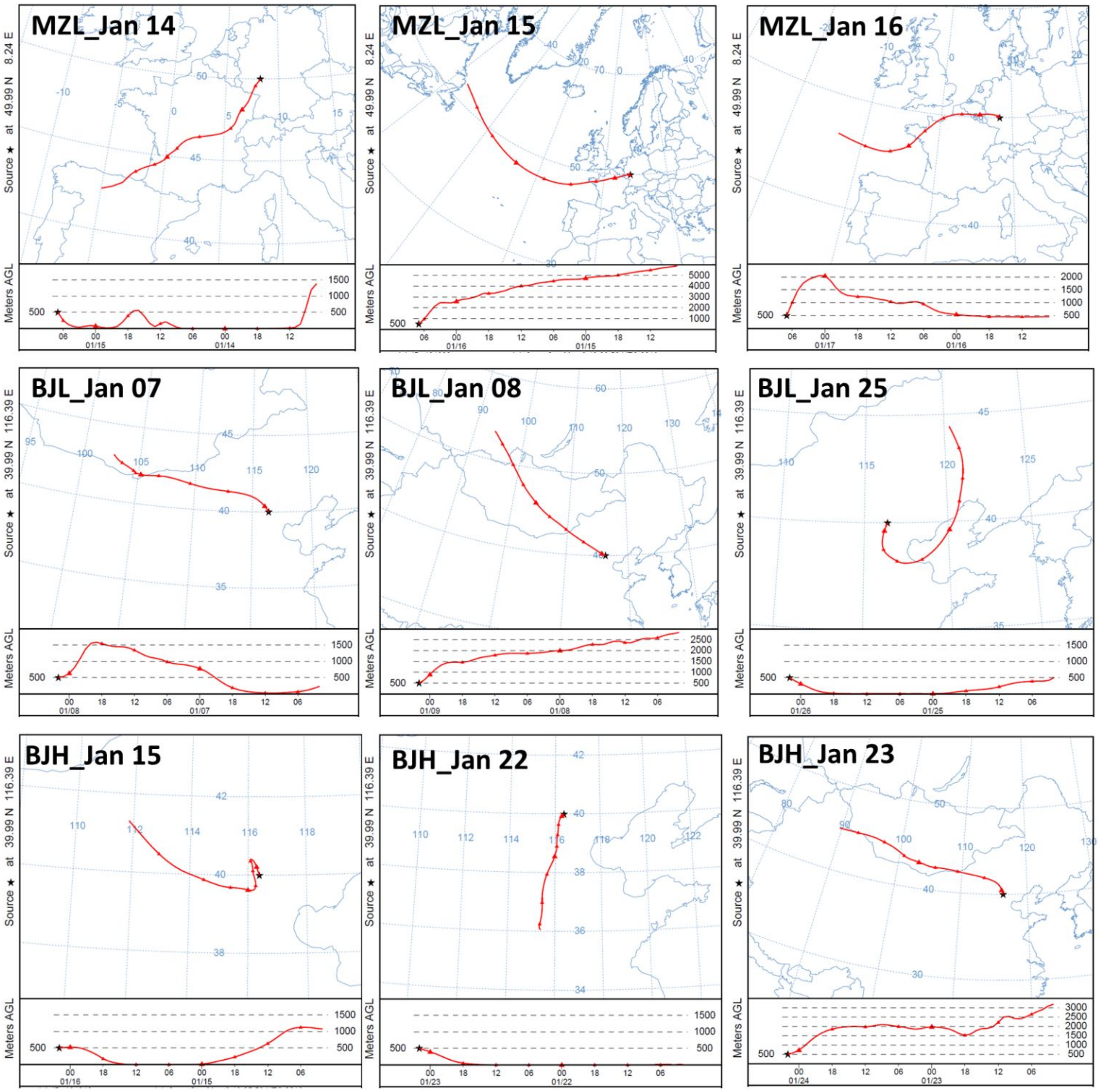

Figure S1. 48 hours back trajectories of air arriving Mainz and Beijing during the sampling time calculated using the NOAA HYSPLIT model.[14]

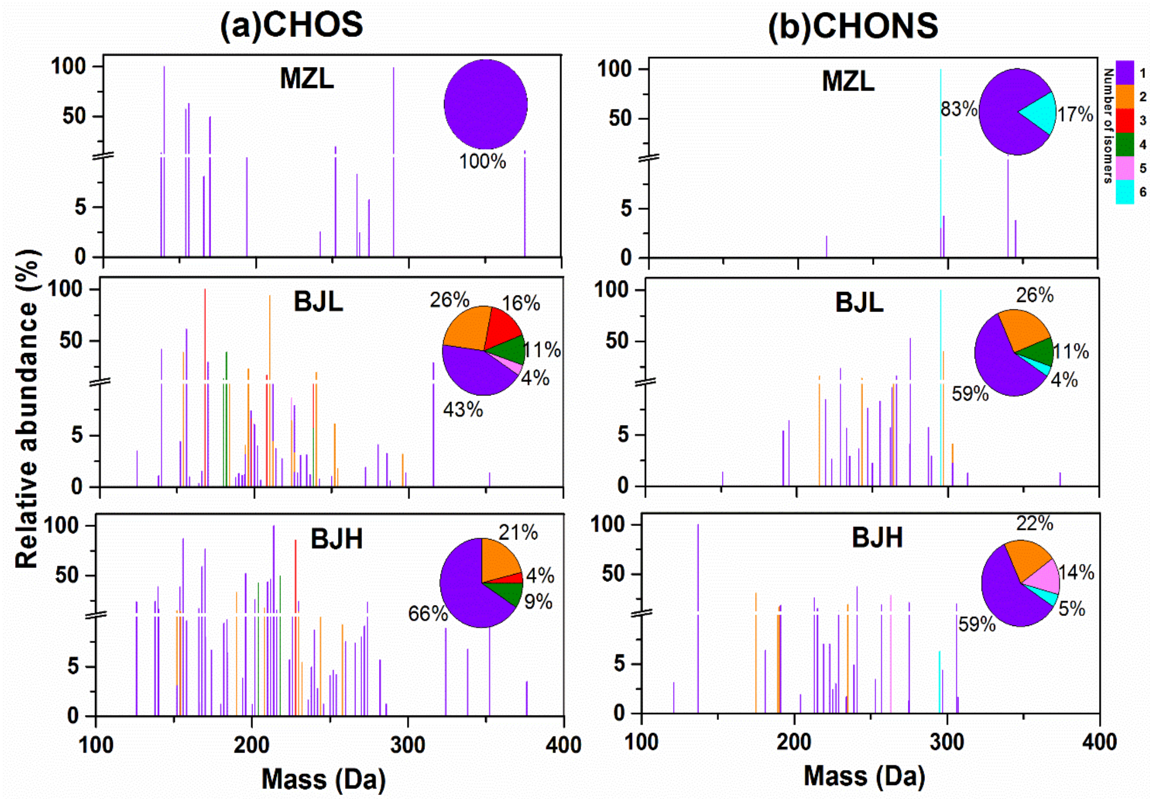

Figure S2. ESI− Orbitrap mass spectra of detected CHOS (a) and CHONS (b) in Mainz and Beijing aerosol samples reconstructed from extracted ion chromatograms. The x-axis corresponds to the molecular mass (Da) of the identified species. The number of isomers for an assigned formula is marked by colors.

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