Complete ozonolysis of alkyl substituted ethenes at –60°C: distributions of ozonide and oligomeric products

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Supporting Information

Fig. 1 Proton NMR spectra of the ozonates recovered upon the complete ozonolysis of, (a) 2,4,4-trimethyl pent-1-ene, **2**, (reaction ***A***) and (b) 2-methyl pent-1-ene, **3**, (reaction ***B***), in pentane at -60°C. **Page 2**

Fig. 2 DEPT carbon NMR spectra of shifts due to the backbone carbons present in the ozonolysis products of (a) 2,3-dimethyl but-2-ene, **1**[6], (b) 3-methylpent-2-ene, **4**, (reaction ***D***) and (c) an equimolar mixture of 2,3-dimethyl but-2-ene, **1**, and 3-methyl pent-2-ene, **4**, (reaction ***E***), in pentane at -60°C; CH/CH_3 resonances depicted upwards, C/CH_2 resonances inverted. **Page 3**

Table 1 Main oligomeric ozonate structures of the ozonolysis of 3-methyl pent-2-ene, **4**, observed from ESI mass spectrometry. **Page 4**

Table 2 Main oligomeric ozonate structures of the ozonolysis of an eqimolar mixture of 2,3-dimethyl but-2-ene, **1**, and 3-methyl pent-2-ene, **4**, observed from ESI mass spectrometry. **Page 5**

Table 3 Main oligomeric ozonate structures of the ozonolysis of *trans* hex-2-ene, **5**, observed from ESI mass spectrometry. **Page 6**

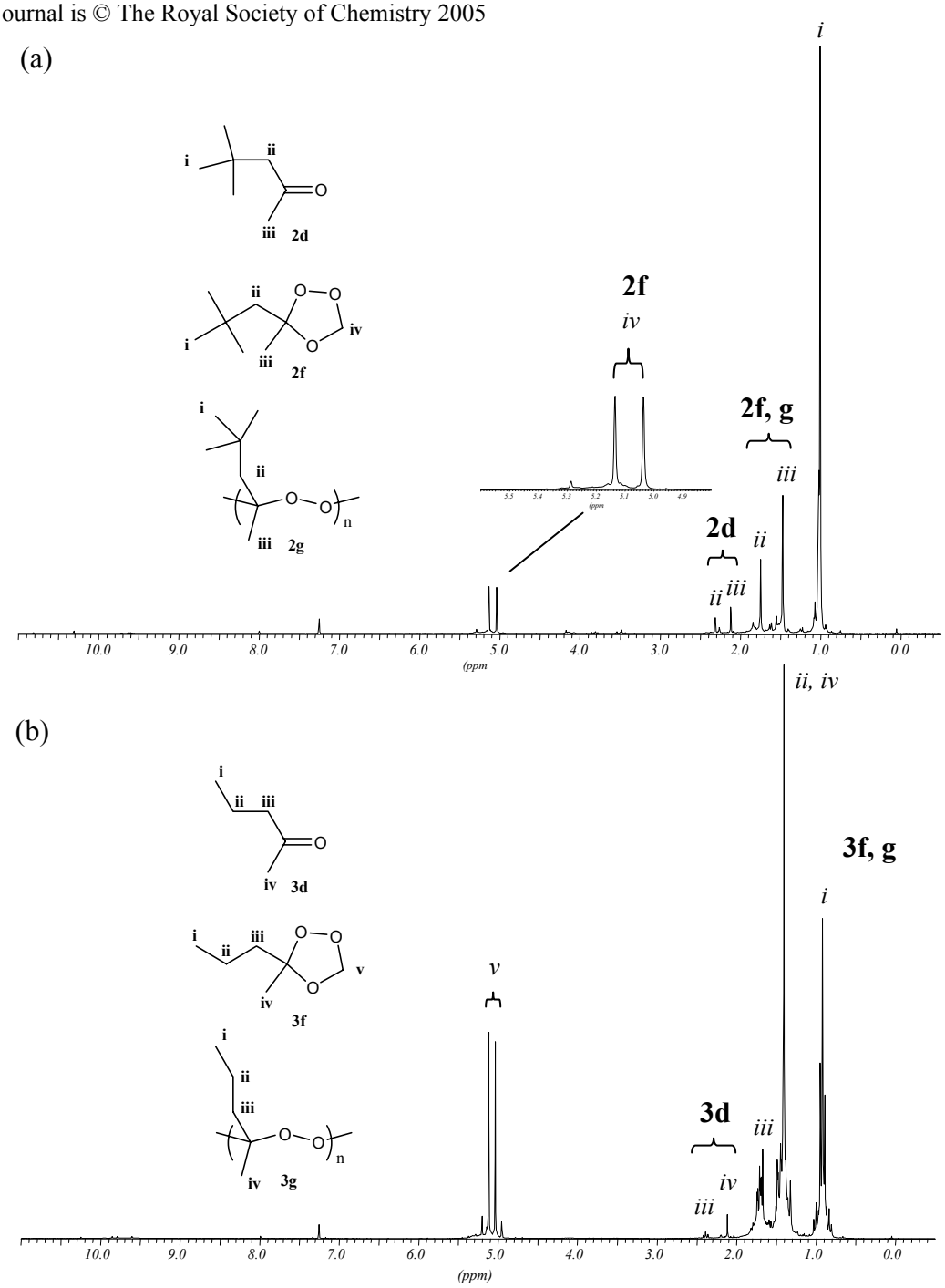


Fig. 1 Proton NMR spectra of the ozonates recovered upon the complete ozonolysis of, (a) 2,4,4-trimethyl pent-1-ene **2** (reaction ***A***) and (b) 2-methyl pent-1-ene **3** (reaction ***B***), in pentane at -60^{o}C.

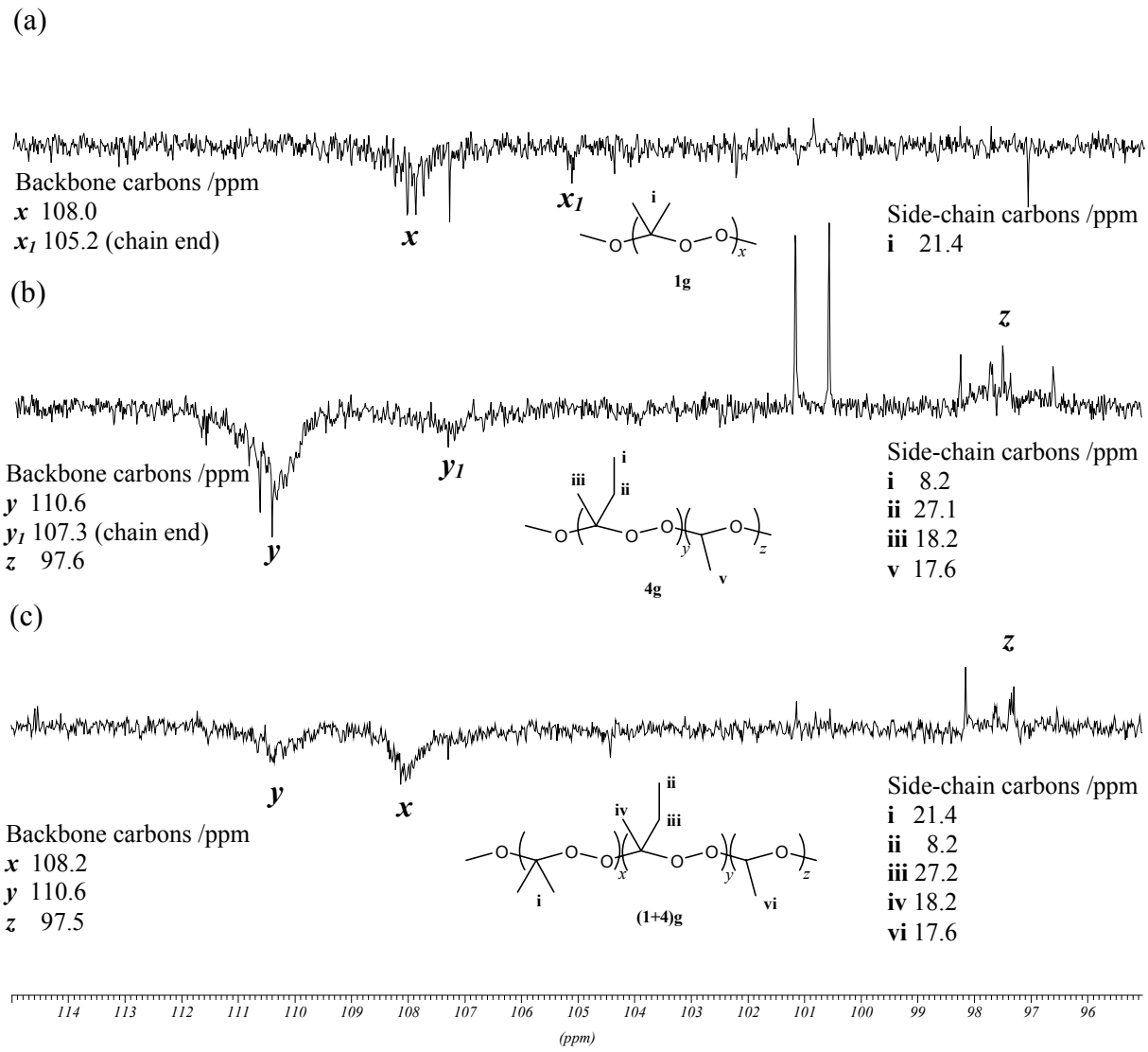


Fig. 2 DEPT carbon NMR spectra of shifts due to the backbone carbons present in the ozonolysis products of (a) 2,3-dimethyl but-2-ene, **1**[6], (b) 3-methyl pent-2-ene, **4**, (reaction ***D***) and (c) an equimolar mixture of 2,3-dimethyl but-2-ene, **1,** and 3-methylpent-2-ene, **4**, (reaction ***E***), in pentane at -60^{o}C; CH/CH_3 resonances depicted upwards, C/CH_2 resonances inverted.

Table 1 Main oligomeric ozonate structures of the ozonolysis of 3-methyl pent-2-ene, **4**, observed from ESI mass spectrometry.

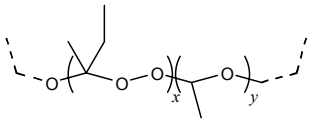
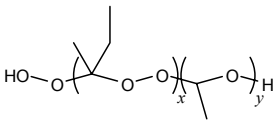
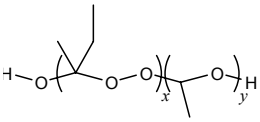
Structure	Molecular ions (m/z) at N = n*x* + n*y* (NH_4^+ adducts)									
n*x* + n*y*	A	B	C	D	E	F	G	H	I	J
★  **4g$_1$**	414	458	502	546	590	634	678	722		
▲  **4g$_2$**		492	536	580	624	668	712	756	800	844
•  **4g$_3$**					608	652	696	740	784	828

Table 2 Main oligomeric ozonate structures of the ozonolysis of an eqimolar mixture of 2,3-dimethyl but-2-ene, **1**, and 3-methyl pent-2-ene, **4**, observed from ESI-MS.

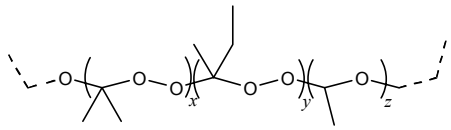
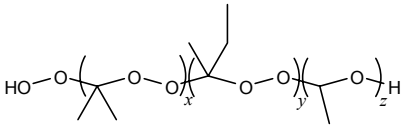
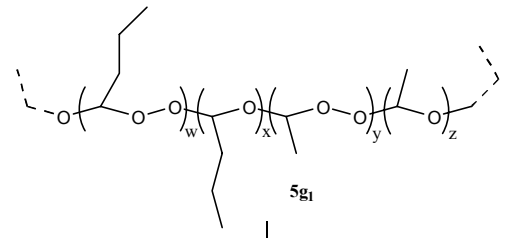
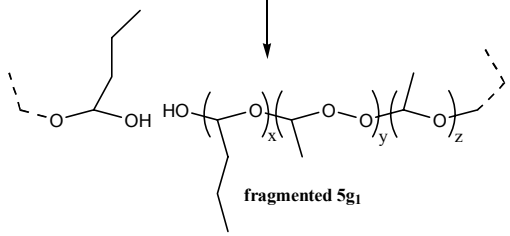
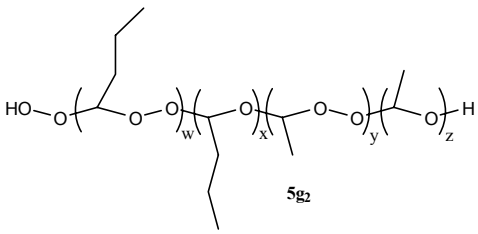
Structure	Molecular ions (m/z) at N = n*x* + n*y* + n*z*					
n*x* + n*y* + n*z*	*x*	*y*	*z*	End groups	NH_4^+	N
 ★ **(1+4)g$_1$**	3	0	4	0	+18	416
	3	1	2	0	+18	416
	3	2	0	0	+18	416
	2	0	6	0	+18	430
	2	1	4	0	+18	430
	2	2	2	0	+18	430
	2	3	0	0	+18	430
	5	0	2	0	+18	476
	5	1	0	0	+18	476
	4	0	4	0	+18	490
	4	1	2	0	+18	490
	4	2	0	0	+18	490
	3	0	6	0	+18	504
	3	1	4	0	+18	504
	3	2	2	0	+18	504
	3	3	0	0	+18	504
	2	0	8	0	+18	518
	2	1	6	0	+18	518
	2	2	4	0	+18	518
	2	3	2	0	+18	518
	2	4	0	0	+18	518
 ▲ **(1+4)g$_2$**	3	0	4	+34	+18	450
	3	1	2	+34	+18	450
	3	2	0	+34	+18	450
	4	0	4	+34	+18	524
	4	1	2	+34	+18	524
	4	2	0	+34	+18	524
	5	0	4	+34	+18	598
	5	1	2	+34	+18	598
	5	2	0	+34	+18	598

Table 3 Main oligomeric ozonate structures of the ozonolysis of *trans* hex-2-ene, **5**, observed from ESI mass spectrometry.

Structure	Molecular ions (m/z) at N = n*w* + n*x* + n*y* + n*z*						
n*w* + n*x* + n*y* + n*z*	*w*	*x*	*y*	*z*	End groups	NH_4^+	N
	1	1	1	0	0	18	238
	2	0	0	1	0	18	238
	0	1	1	2	0	18	238
	1	0	0	3	0	18	238
	0	0	0	5	0	18	238
 **$5g_1$**	3	1	1	0	2	18	416
	0	**3**	**3**	**0**	**2**	**18**	**416***
	4	0	0	1	2	18	416
 **fragmented $5g_1$**	**1**	**2**	**2**	**1**	**2**	**18**	**416***
	2	**1**	**1**	**2**	**2**	**18**	**416***
	3	**0**	**0**	**3**	**2**	**18**	**416***
	0	2	2	3	2	18	416
	1	1	1	4	2	18	416
	2	0	0	5	2	18	416
	0	1	1	6	2	18	416
	1	0	0	7	2	18	416
	0	0	0	9	2	18	416
 **$5g_2$**	1	3	1	0	34	18	416
	2	2	0	1	34	18	416
	0	3	1	2	34	18	416
	1	2	0	3	34	18	416
	0	2	0	5	34	18	416

*Structures highlighted in bold are most likely to contribute to the 416 ion given the proton NMR analysis of the ozonate mixture.