

Supporting information: List of the toxaphene pool fractions, their $>C=C<$ valence bonds and corresponding structural assignment

No. of the pool fraction	Fraction intervals	Total amount		Trans- mission	$\bar{\nu}_{C=C}$ [cm^{-1}] (bold: main absorption band)	Chlorobornenes [mg]				Chlorocamphenes [mg]			
		[mg]	[%]						Σ				Σ
1	131-150	4.4	0.088	-	-	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	151-170	4.0	0.080	-	-	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
3	171-180	5.0	0.100	-	-	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	181-190	5.1	0.102	-	-	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
5	191-200	4.1	0.082	-	-	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
6	201-220	9.4	0.188	91	1605, 1585	0.8	0.0	0.6	1.4	0.0	0.0	0.0	0.0
7	221-230	14.0	0.280	81	1610, 1590, 1641	1.0	0.0	0.5	1.5	0.0	0.7	0.0	0.0
8	231-240	29.5	0.590	40	1608, 1591	1.5	0.0	2.3	3.8	0.0	0.0	0.0	0.0

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		[mg]	[%]						Σ				Σ
9	241-260	115.8	2.316	5	1608	0.0	0.0	16.5	16.5	0.0	0.0	0.0	0.0
10	261-280	62.2	1.244	47	1608, 1617	0.0	0.0	2.0	2.0	1.5	0.0	0.0	1.5
11	281-300	56.5	1.130	69	1620, 1627, 1595	0.0	0.7	0.0	0.7	2.7	0.0	0.0	2.7
12	301-320	84.2	1.684	68	1621, 1608, 1642	0.0	0.0	0.8	0.8	3.2	0.8	0.0	4.0
13	321-349	137.4	2.748	59	1607, 1632, 1622	0.0	0.0	13.1	13.1	1.1	1.7	0.0	1.8
14	350-370	97.0	1.940	65	1620, 1610, 1645	0.0	<0.1	7.2	7.2	2.0	1.5	0.0	3.5
15	371-399	128.2	2.564	65	1621, 1608, 1644	0.0	0.0	8.0	8.0	3.2	1.7	0.0	4.9
16	400-410	57.0	1.140	85	1620, 1608, 1644	0.0	0.0	3.2	3.2	1.1	0.3	0.0	1.4
17	411-419	44.2	0.884	85	1630, 1607, 1642	0.0	0.0	2.3	0.0	?	2.2	0.0	2.2
18	420-439	110.7	2.214	70	1630, 1644, 1620	0.4	<0.1	0.0	0.4	2.1	4.5	0.0	6.6
19	440-459	139.4	2.788	70	1630, 1644, 1618	0.4	<0.1	0.0	0.4	1.9	5.2	0.0	7.1

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		[mg]	[%]						Σ				Σ
20	460-469	85.3	1.706	80	1644, 1632, 1615	0.3	<0.1	0.0	0.3	0.9	2.7	0.0	3.6
21	470-500	218.2	4.364	60	1632, 1644, 1613	1.6	<0.1	0.0	1.6	4.5	15.0	0.0	9.5
22	501-530	191.0	3.820	60	1632, 1644, 1616	0.0	0.0	<0.1	<0.1	2.7	7.8	0.0	10.5
23	531-550	105.6	2.112	75	1633, 1644, 1616	0.0	0.0	<0.1	<0.1	0.8	3.9	0.0	4.7
24	551-580	145.4	2.910	70	1633, 1616	0.0	0.0	<0.1	<0.1	1.1	6.3	0.0	7.4
25	581-599	87.0	1.740	80	1632, 1618, 1651	0.0	0.0	0.0	0.0	0.6	3.8	0.5	4.9
26	600-629	142.6	2.852	86	1632, 1644	0.0	0.0	0.0	0.0	0.0	5.9	<0.1	5.9
27	630-659	134.5	2.690	88	1632, 1617, 1641	0.0	0.0	<0.1	<0.1	1.2	4.8	0.0	6.0
28	660-669	57.2	1.144	90	1631, 1642, 1617	0.0	0.0	<0.1	<0.1	0.3	2.1	0.0	2.4
29	670-679	46.0	0.920	92	1632, 1644, 1617	0.0	0.0	0.0	0.0	0.2	0.9	0.0	1.1
30	680-689	41.8	0.836	93	1644, 1633, 1614	0.0	0.0	0.0	0.0	<0.1	0.8	0.0	0.8

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		[mg]	[%]						Σ				Σ
31	690-709	105.0	2.100	85	1647, 1633, 1597	0.0	0.0	0.5	0.5	0.0	0.0	4.0	4.0
32	710-730	119.7	2.394	88	1647, 1633, 1596	0.0	0.0	0.8	0.8	0.0	0.0	4.3	4.3
33	731-780	231.2	4.624	88	1646, 1633, 1596	0.0	0.0	1.9	1.9	0.0	0.0	7.9	7.9
34	781-799	73.0	1.460	90	1646, 1632, 1613	0.0	0.0	<0.1	<0.1	0.8	2.7	0.0	2.5
35	800-809	39.6	0.792	91	1646, 1615, 1596	0.0	0.0	0.3	0.3	0.4	1.5	0.0	1.9
36	810-829	78.4	1.568	82	1647, 1617, 1652	0.0	0.0	<0.1	<0.1	0.3	2.8	1.0	4.1
37	830-839	44.8	0.896	88	1647, 1617, 1651	0.0	0.0	<0.1	<0.1	0.2	1.3	0.5	2.0
38	840-910	200.6	4.012	83	1646, 1652, 1596	0.0	0.0	2.0	2.0	0.0	8.0	1.3	9.3
39	911-929	42.8	0.856	90	1646, 1630, 1652	0.0	0.0	<0.1	<0.1	0.0	0.9	0.3	1.2
40	930-949	36.6	0.732	90	1646, 1635, 1652	0.0	0.0	<0.1	<0.1	0.0	0.7	0.2	0.9
41	950-969	32.0	0.640	92	1633, 1612, 1646	0.0	0.0	<0.1	<0.1	0.0	0.6	<0.1	0.6

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		[mg]	[%]						Σ				Σ
42	970-980	16.8	0.336	95	1646, 1635, 1652	0.0	0.0	0.0	0.0	0.0	0.3	0.2	0.5
43	981-1029	73.4	1.468	80	1634, 1652, 1601	0.0	0.0	0.7	0.7	0.0	1.4	0.4	1.8
44	1030-1059	45.3	0.906	78	1634, 1656, 1646	0.0	0.0	0.0	0.0	0.0	0.8	0.2	1.0
45	1060-1080	29.3	0.586	93	1634, 1656, 1646	0.0	0.0	0.0	0.0	0.0	0.5	<0.1	0.5
46	1081-1089	14.3	0.286	93	1635, 1652, 1646	0.0	0.0	0.0	0.0	0.0	0.2	<0.1	0.2
47	1090-1109	27.1	0.542	94	1635, 1652, 1646	0.0	0.0	0.0	0.0	0.0	0.6	<0.1	0.6
48	1110-1149	58.0	1.160	88	1636, 1652, 1646	0.0	0.0	0.0	0.0	0.0	1.2	0.2	1.4
49	1150-1179	30.8	0.616	88	1635, 1652, 1646	0.0	0.0	0.0	0.0	0.0	0.8	0.1	0.9
50	1180-1190	9.3	0.186	94	1635, 1627, 1652	0.0	0.0	0.0	0.0	0.1	0.2	0.1	0.4
51	1191-1200	7.0	0.140	96	1635, 1629, 1652	0.0	0.0	0.0	0.0	<0.1	0.2	0.1	0.3
52	1201-1220	13.0	0.260	91	1635, 1629, 1652	0.0	0.0	0.0	0.0	<0.1	0.1	0.1	0.2

No. of the pool fraction	Fraction intervalls	Total amount		Trans- mission	$\bar{\nu}_{\text{C=C}}$ [cm ⁻¹] (bold: main absorption band)	Chlorobornenes [mg]				Chlorocamphenes [mg]			
		[mg]	[%]						Σ				Σ
53	1221-1250	16.6	0.332	88	1635, 1629, 1652	0.0	0.0	0.0	0.0	<0.1	0.1	0.1	0.2
54	1251-1279	14.5	0.290	87	1635, 1629, 1652	0.0	0.0	0.0	0.0	<0.1	0.1	0.1	0.2
55	1280-1289	6.0	0.120	96	1633, 1618, 1644	0.0	0.0	0.0	0.0	0.1	0.1	0.0	0.2
56	1290-1309	11.4	0.228	91	1633, 1644, 1618	0.0	0.0	0.0	0.0	0.1	0.1	0.0	0.2
57	1310-1329	8.9	0.178	92	1635, 1645, 1652, 1618	0.0	0.0	0.0	0.0	0.1	0.1	0.0	0.2
58	1330-1349	12.0	0.240	93	1635, 1645, 1618	0.0	0.0	0.0	0.0	0.2	0.1	0.0	0.3
59	1350-1369	8.4	0.168	93	1646, 1635, 1599	0.0	0.0	0.2	0.2	0.0	0.2	0.0	0.2
60	1370-1389	7.2	0.144	93	1647, 1636, 1596	0.0	0.0	0.2	0.2	0.0	0.2	0.0	0.2
61	1390-1419	11.8	0.236	93	1645, 1634, 1601	0.0	0.0	0.2	0.2	0.0	0.1	0.0	0.1
62	1420-1449	10.6	0.282	94	1645, 1630, 1597	0.0	0.0	0.2	0.2	0.0	0.2	0.0	0.2

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		[mg]	[%]						Σ				Σ
63	1450-1479	10.4	0.208	93	1645, 1633, 1596	0.0	0.0	0.1	0.1	0.0	0.2	0.0	0.2
64	1480-1510	10.4	0.208	92	1646, 1596, 1615	0.0	0.0	0.0	0.0	0.1	0.2	0.0	0.3
65	1511-1550	12.0	0.240	92	1645, 1596	0.0	0.0	0.1	0.1	0.0	0.2	0.0	0.1
66	1551-1579	8.9	0.480	90	1645, 1596	0.0	0.0	0.1	0.1	0.0	0.1	0.0	0.1
67	1580-1599	7.0	0.140	92	1646, 1636, 1596	0.0	0.0	0.1	0.1	0.0	0.1	0.0	0.1
68	1600-1609	2.8	0.056	95	1646, 1636	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
69	1610-1629	6.2	0.124	92	1646, 1636	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
70	1630-1639	3.3	0.066	96	-	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
71	1640-1669	10.8	0.216	90	1646	0.0	0.0	0.0	0.0	0.0	0.2	0.0	0.2
72	1670-1770	43.1	0.862	87	1646, 1635	0.0	0.0	0.0	0.0	0.0	1.1	0.0	1.1
73	1771-1810	12.9	0.258	88	1646	0.0	0.0	0.0	0.0	0.0	0.3	0.0	0.3

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		[mg] [%]	[%]					Σ				Σ
74	1811-1820	2.3 0.046	96	-	0.0	0.0	0.0	0.0	2.0	0.0	0.0	2.0
75	1821-1849	6.6 0.132	93	1645	0.0	0.0	0.0	0.0	0.1	0.0	0.0	0.1
76	1850-1879	6.4 0.178	92	1646	0.0	0.0	0.0	0.0	0.1	0.0	0.0	0.1
77	1880-1919	7.1 0.142	92	1646	0.0	0.0	0.0	0.0	0.1	0.0	0.0	0.1
78	1920-1939	4.9 0.098	94	-	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
79	1940-1979	10.7 0.214	90	1646	0.0	0.0	0.0	0.0	0.2	0.0	0.0	0.2
80	1980-2000	4.2 0.084	94	1646, 1636	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
81	2001-2039	5.8 0.116	92	1644, 1633	0.0	0.0	0.0	0.0	<0.1	0.0	0.0	0.0
82	2040-2060	1.8 0.036	94	1644	0.0	0.0	0.0	0.0	<0.1	0.0	0.0	0.0
83	2061-2109	3.8 0.076	89	1645	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
84	2110-2129	0.7 0.014	96	1632	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

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		[mg]	[%]						Σ				Σ
85	2130-2149	1.4	0.018	96	1632	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
86	2150-2169	9.1	0.182	96	1632	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.1
87	2170-2189	14.2	0.284	96	1632	0.0	0.0	0.0	0.0	0.0	1.3	0.0	1.3
88	2190-2239	8.4	0.168	93	1633, 1610	0.0	0.0	0.0	<0.1	0.0	<0.1	0.0	0.0
89	2240-2270	9.8	0.196	96	1642, 1610	0.0	0.0	0.0	<0.1	0.0	<0.1	0.0	0.0
90	2271-2289	3.8	0.076	96	1642, 1610	0.0	0.0	0.0	<0.1	0.0	<0.1	0.0	0.0
91	2290-2310	5.8	0.116	98	1649, 1605, 1633	-	-	-	<0.1	-	<0.1	-	-
92	2311-2329	4.9	0.098	98	1633, 1642	-	0.0	0.0	0.0	0.0	<0.1	0.0	0.0
93	2330-2350	4.2	0.084	98	1631, 1641	0.0	0.0	0.0	0.0	0.0	<0.1	0.0	0.0
94	2351-2380	4.0	0.080	97	1640, 1631	0.0	0.0	0.0	0.0	0.0	<0.1	0.0	0.0
95	2381-2399	0.7	0.014	88	1632, 1642	0.0	0.0	0.0	0.0	0.0	0.2	0.0	0.2

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		[mg] [%]	[%]		Σ	Σ
96	2400-2409	7.7 0.154	96	1635 , 1652	0.0 0.0	0.0 0.0
97	2410-2419	3.9 0.078	97	1635 , 1652	0.0 0.0	0.0 0.0
98	2420-2429	5.4 0.108	98	1635 , 1652	0.0 0.0	0.0 0.0
99	2430-2439	4.2 0.084	97	1635 , 1652	0.0 0.0	0.0 0.0
100	2440-2459	4.6 0.092	96	1615 , 1652	0.0 0.0	0.0 0.0
101	2460-2479	6.7 0.134	96	1635 , 1653	0.0 0.0	0.0 0.0
102	2480-2489	7.4 0.148	98	1635 , 1653	0.0 0.0	0.0 0.0
103	2490-2500	5.0 0.100	97	1635 , 1653	0.0 0.0	0.0 0.0
Methanolfraction in mg		493.7 [9.874]	-	-	0.0 0.0	0.0 0.0
[%]						

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		[mg]	[%]						Σ				Σ
Non extract. comp. in mg [%]		415.6 [8.312]		-	-	-	-	-	-	-	-	-	-
Σ in mg		5000.0				6.0	0.7	61.82	68.52	33.40	118.7	5.6	157.7
Σ in %		100				0.12	0.014	1.236	1.370	0.67	2.374	0.112	3.154