

## Reagent Chemicals

Ninth Edition

### ACS Specifications

Official from January 1, 2000  
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Reagent: **Organochlorine  
Pesticides**

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## Organochlorine Pesticides

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### REQUIREMENTS

#### *Identity by*

Infrared spectroscopy . . . . . Passes test

Gas chromatography/mass spectrometry . . . . . Passes test

#### *Assay by*

Gas chromatography . . . . .  $\geq 98.0\%$

Thin-layer chromatography . . . . . Passes test

#### *Specific Use*

GC-ECD suitability . . . . . Passes test

### TESTS

**IDENTITY BY INFRARED SPECTROSCOPY.** Analyze the sample using the general procedure cited on page 79. Identifying absorbances for the compound listed in Table XV must be present. The spectrum is compared to the NIST standardized library of compounds, if available. Absorbances in the test spectrum must match those found in the NIST spectrum.

**IDENTITY BY GAS CHROMATOGRAPHY/MASS SPECTROMETRY.** Analyze the sample by gas chromatography/mass spectrometry using method GCMS-OCP1 described below.

#### *Method GCMS-OCP1*

**Ionization Mode:** Electron ionization/70eV

**Column:** 5% Diphenyl–95% dimethylpolysiloxane, 30 M  $\times$  0.25 mm i.d., 0.25  $\mu$ m film thickness

**Temperature Program:** 45 °C for 1 min, then 10 °C/min to 300 °C, hold 10 min

**Carrier Gas:** Helium at 1.0 mL/min

**Injector:** Split/splitless (100:1 split)

**Injector Temperature:** 250 °C

**Scan Range:** 33–525 amu

**Sample Size:** 1  $\mu$ L of a 500  $\mu$ g/mL solution

Identifying ions for the compound listed in Table XV must be present. The spectrum is compared to the NIST standardized library of compounds, if available. Ions in the test spectrum must match those found in the NIST spectrum.

**ASSAY BY GAS CHROMATOGRAPHY.** Analyze the sample by gas chromatography using method GC-OCP1 described below.

#### *Method GC-OCP1*

**Column:** 5% Diphenyl–95% dimethylpolysiloxane, 30 M  $\times$  0.53 mm i.d., 1.0  $\mu$ m film thickness

**Detector:** Flame ionization

**Detector Temperature:** 200 °C

**Injector:** Splitless

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**Injector Temperature:** 200 °C

**Sample Size:** 2 µL of a 1000 µg/mL solution

**Carrier Gas:** Helium at 3.0 mL/min

**Temperature Program:** 70 °C, then 5 °C/min to 210 °C, hold 10 min

Measure the area under all peaks (excluding the solvent peak) and calculate the analyte content in area percent.

**ASSAY BY THIN LAYER CHROMATOGRAPHY.** Analyze the sample by thin layer chromatography using the general procedure described on page 73. The following specific conditions are also required.

**Stationary Phase:** Silica

**Mobile Phase:** Hexane

**Detection Method:** UV at 254 nm and iodine

Compound must exhibit a single spot.

**GC-ECD SUITABILITY.** Prepare a 200 ng/mL solution of the sample in an ECD nonresponsive solvent. Analyze the sample using method GC-OCP2 described below.

#### *Method GC-OCP2*

**Column:** 5% Diphenyl-95% dimethylpolysiloxane, 30 M × 0.53 mm i.d., 1.5 µm film thickness

**Detector:** Electron capture

**Detector Temperature:** 325 °C

**Injector:** Splitless

**Injector Temperature:** 250 °C

**Sample Size:** 1 µL

**Carrier Gas:** Nitrogen at 3.5 mL/min

**Temperature Program:** 45 °C for 1 min, then 10 °C/min to 250 °C, hold 10 min

Measure the area under all peaks (excluding the solvent peak) and calculate the analyte and total impurities content in area percent. The sum of all impurity peaks should not exceed 5%, with no single peak greater than 3%.

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**Table XV. Organochloride Pesticides Compound Data**

Name	CAS No.	Chemical Formula	Formula Weight	IR ( $cm^{-1}$ )			MS ( $m/z$ )		
				IR-1	IR-2	IR-3	MS-1	MS-2	MS-3
Aldrin	309-00-2	C <sub>12</sub> H <sub>8</sub> Cl <sub>6</sub>	364.91	2987	1597	693	66	362	263
<i>a</i> -BHC	319-84-6	C <sub>6</sub> H <sub>6</sub> Cl <sub>6</sub>	290.83	2963	1340	793	183	219	181
<i>b</i> -BHC	319-85-7	C <sub>6</sub> H <sub>6</sub> Cl <sub>6</sub>	290.83	2952	1309	754	109	253	181
<i>d</i> -BHC	319-86-8	C <sub>6</sub> H <sub>6</sub> Cl <sub>6</sub>	290.83	2932	1236	774	109	219	183
<i>g</i> -BHC	58-89-9	C <sub>6</sub> H <sub>6</sub> Cl <sub>6</sub>	290.83	2948	1344	689	181	288	219
Butachlor	23184-66-9	C <sub>17</sub> H <sub>26</sub> ClNO <sub>2</sub>	311.85	2971	1703	1074	176	311	57
<i>cis</i> -Chlordane	5103-71-9	C <sub>10</sub> H <sub>6</sub> Cl <sub>8</sub>	409.78	2963	1604	534	373	406	272
<i>trans</i> -Chlordane	5103-74-2	C <sub>10</sub> H <sub>6</sub> Cl <sub>8</sub>	409.78	2964	1603	560	373	406	272
Chlordecone	143-50-0	C <sub>10</sub> Cl <sub>10</sub> O	490.63	1814	1043	646	272	274	237
Chlorobenzilate	510-15-6	C <sub>16</sub> H <sub>14</sub> Cl <sub>2</sub> O <sub>3</sub>	325.20	3495	1719	1485	251	139	111
Chloroneb	2675-77-6	C <sub>8</sub> H <sub>8</sub> Cl <sub>2</sub> O <sub>2</sub>	207.05	2950	1490	775	191	206	141
Chlorthal	1861-32-1	C <sub>10</sub> H <sub>6</sub> Cl <sub>4</sub> O <sub>4</sub>	331.96	2963	1762	1240	301	330	299
2,4'-DDD	53-19-0	C <sub>14</sub> H <sub>10</sub> Cl <sub>4</sub>	320.04	3075	1490	770	235	318	165
4,4'-DDD	72-54-8	C <sub>14</sub> H <sub>10</sub> Cl <sub>4</sub>	320.04	3090	1494	765	235	318	165
2,4'-DDE	3424-82-6	C <sub>14</sub> H <sub>8</sub> Cl <sub>4</sub>	318.02	3075	1590	862	246	316	248
4,4'-DDE	72-55-9	C <sub>14</sub> H <sub>8</sub> Cl <sub>4</sub>	318.02	3090	1490	858	246	316	248
2,4'-DDT	789-02-6	C <sub>14</sub> H <sub>9</sub> Cl <sub>5</sub>	354.48	3075	1490	777	335	352	165
4,4'-DDT	50-29-3	C <sub>14</sub> H <sub>9</sub> Cl <sub>5</sub>	354.48	3094	1494	774	235	352	165
Dibutylchloredate	1770-80-5	C <sub>17</sub> H <sub>20</sub> Cl <sub>6</sub> O <sub>4</sub>	501.06	2960	1745	845	501	499	427
Dicamba	1918-00-9	C <sub>8</sub> H <sub>6</sub> Cl <sub>2</sub> O <sub>3</sub>	221.04	3565	1776	1167	173	220	175
Diclorofop methyl	51338-27-3	C <sub>16</sub> H <sub>14</sub> Cl <sub>2</sub> O <sub>4</sub>	341.20	3000	1750	1219	253	340	281
Dicofol	115-32-2	C <sub>14</sub> H <sub>9</sub> Cl <sub>5</sub> O	370.50	3532	805	770	139	251	111
Dieldrin	60-57-1	C <sub>12</sub> H <sub>8</sub> Cl <sub>6</sub> O	380.91	2986	1599	850	79	378	263
Endosulfan I	959-98-8	C <sub>9</sub> H <sub>6</sub> Cl <sub>6</sub> O <sub>3</sub> S	406.93	2937	1605	752	195	404	339
Endosulfan II	33213-65-9	C <sub>9</sub> H <sub>6</sub> Cl <sub>6</sub> O <sub>3</sub> S	406.92	2959	1205	673	195	404	339
Endosulfan sulfate	1031-07-8	C <sub>9</sub> H <sub>6</sub> Cl <sub>6</sub> O <sub>4</sub> S	422.93	1437	1201	808	272	420	387
Endrin	72-20-8	C <sub>12</sub> H <sub>8</sub> Cl <sub>6</sub> O	380.91	2979	1600	855	81	378	263
Endrin aldehyde	7421-93-4	C <sub>12</sub> H <sub>8</sub> Cl <sub>6</sub> O	380.91	2940	1741	835	67	345	250
Endrin ketone	53494-70-5	C <sub>12</sub> H <sub>7</sub> Cl <sub>6</sub> O	380.91	2963	1748	754	317	378	250
Heptachlor	76-44-8	C <sub>10</sub> H <sub>5</sub> Cl <sub>7</sub>	373.32	2959	1602	789	100	370	272
Heptachlor epoxide	1024-57-3	C <sub>10</sub> H <sub>5</sub> Cl <sub>7</sub>	389.32	3044	1602	858	81	386	353
Hexachlorophene	70-30-4	C <sub>13</sub> H <sub>6</sub> Cl <sub>6</sub> O <sub>2</sub>	406.90	3502	1438	1281	196	404	209
Isodrin	465-73-6	C <sub>12</sub> H <sub>8</sub> Cl <sub>6</sub>	364.91	2963	1603	1468	193	362	263
Mecoprop	7085-19-0	C <sub>10</sub> H <sub>11</sub> ClO <sub>3</sub>	214.65	3575	1803	1490	142	214	107
Metolachlor	51218-45-2	C <sub>15</sub> H <sub>22</sub> ClNO <sub>2</sub>	283.79	2982	1691	1113	162	238	146
Mirex	2385-85-5	C <sub>10</sub> Cl <sub>12</sub>	545.54	1148	1059	650	272	274	237
4,4'-Methoxychlor	72-43-5	C <sub>16</sub> H <sub>15</sub> Cl <sub>3</sub> O <sub>2</sub>	345.65	2938	1511	1252	227	344	228
<i>cis</i> -Nonachlor	5103-73-1	C <sub>10</sub> H <sub>5</sub> Cl <sub>9</sub>	444.23	2980	1599	1267	409	440	237
<i>trans</i> -Nonachlor	39765-80-5	C <sub>10</sub> H <sub>5</sub> Cl <sub>9</sub>	444.23	2954	1599	1257	409	440	272
Pentachloroanisole	1825-21-4	C <sub>7</sub> H <sub>3</sub> Cl <sub>5</sub> O	280.36	2948	1375	1032	280	278	265
Propachlor	1918-16-7	C <sub>11</sub> H <sub>14</sub> ClNO <sub>4</sub>	211.69	2982	1691	704	120	211	176