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Gibbs Free Energy of Formation of Chlordecone and Potential Degradation Products: Implications for Remediation Strategies and Environmental Fate

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This paper is dedicated in memoriam of Yves-Marie Cabidoche pioneer in the study of the chlordecone problem in the FWI

ABSTRACT: Chlordecone ($C_{10}Cl_{10}O$; CAS number 143-50-0) has been used extensively as an organochlorine insecticide, but is nowadays banned under The Stockholm Convention on Persistent Organic Pollutants (POPs). A search for chlordecone respiring organisms and choosing between reductive versus oxidative remediation tools and strategies to clean up chlordecone polluted environments would benefit from the availability of Gibbs free energy data of chlordecone and its potential dechlorination products. Presently such data are not available. Polycyclic "cage" molecules of which chlordecone is an example contain considerable strain energy. It is not a priory clear how this affects thermodynamic properties of the chlorinated members of this unique class of compounds, and to what extent redox potentials for the halogenated congeners are different from those of other aliphatic and aromatic organohalogens. We have performed *ab initio* quantum chemical calculations to estimate $\Delta_f H_m^o$ and $\Delta_f G_m^o$ values of chlordecone and selected dechlorination products, and used these data to calculate their Gibbs free energy and redox potential. With redox potentials in the range of 336 to 413 mV chlordecone has an E_o' value similar to that of other organochlorines. The results indicate that there are no thermodynamic reasons why chlordecone respiring or fermenting organisms should not exist.

INTRODUCTION

Chlordecone ($C_{10}Cl_{10}O$; CAS number 143-50-0) (Figure 1) is an organochlorine pesticide with all the salient characteristics that have given this class of compounds its deservedly bad reputation. It sorbs strongly to soils, is poorly soluble in water, and highly persistent in the environment; it accumulates in food chains, has potent chronic and acute toxicity, and is a proven carcinogen.[1,2] Patented as an insecticide in 1952 (US Patent

2,616,928) it was produced for Allied Chemical Corporation in Hopewell, VA, between 1966 and 1975, mainly for the export to tropical countries where it was used against a wide range of pests, and to Germany where it was converted into Kelevan and used against the Colorado beetle.[3,4] The production in Hopewell was managed poorly: many of

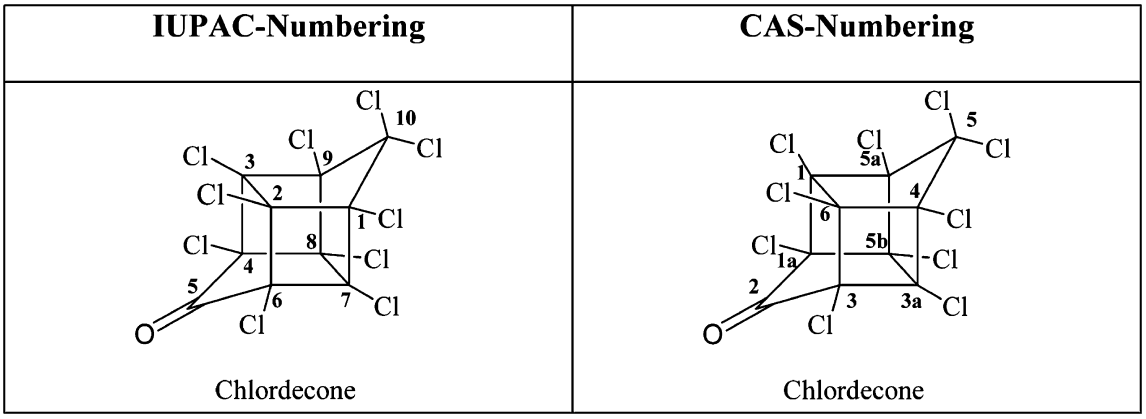

Figure 1. Chlordecone; carbons numbered according to the IUPAC and the CAS nomenclatures.

the laborers developed acute toxicity symptoms, the soils around the plant got severely polluted with chlordecone, and the James River in which the wastewater was discharged after passage through the municipal sewage treatment works had to be closed for the harvest of shellfish and finfish for a period of 18 years.[5-7] The plants in Hopewell were closed in 1975, and manufacturing and use of chlordecone was forbidden in the US from 1977 onwards.[3,4] Production of chlordecone moved to Brazil. The active agent was exported from Brazil to France where it was formulated into Curlone (dust with 5% w/w chlordecone) until the WHO proposed a worldwide ban on its use.[8] Chlordecone is now banned under The Stockholm Convention on Persistent Organic Pollutants (POPs), a global treaty under auspices of the United Nations[9], and classifies as legacy POP with all the negative connotations that the word invokes.[10] For example, chlordecone has been intensively used on the French islands of Martinique and Guadeloupe between 1972 and 1993 against the banana weevil *Cosmopolites sordidus*; this has resulted in long term pollution of soils and contamination of waters, aquatic biota and crops.[11-15] Its slow dissipation from the volcanic soils on the islands is ascribed to leaching via drainage water, and a significant part of the original dose ends up in sediments and fish and crustaceans on the islands. [12,14] History repeats itself, and consumption of fish and crustacean caught on or nearby some parts of the islands is forbidden.[14] Recent data show that chlordecone is present in the blood of adult men, pregnant women, and newborns in Guadeloupe.[16-18] Main contributors to chlordecone exposure include seafood, root vegetables, and *Cucurbitaceae.*[19] Thus, there is growing political and social pressure to find remediation solutions to the chlordecone problem on the French West Indies (FWI). Bioremediation, alone or in combination with physicochemical approaches, could be one of the options. The high chlorine content of the chlordecone molecule (Figure 1) makes anaerobic dechlorination the most likely mode of initial attack[20]: a wide series of different aromatic and aliphatic compound classes are susceptible to reductive dechlorination, including chlorinated ethylenes, PCBs and dioxins.[21,22]

After the Hopewell disaster in the 1970s there has been a short-lived flurry of research into the environmental fate of chlordecone including some work on biodegradation, funded by the fines levied on Allied Chemicals.[23] Orndorff and Colwell have performed experiments under aerobic conditions and detected potential degradation products of chlordecone, but limited to the removal of 1 or 2 chlorine atoms from the carbon backbone.[24] Experiments conducted under anaerobic conditions[25,26] were more promising. Schrauzer and Katz[25] used vitamin B_{12S} and showed that this coenzyme can dechlorinate chlordecone and can induce opening of the bishomocubane "cage". Jablonski et al. subsequently showed that a pure culture of acetate-grown *Methanosarcina thermophila* can convert chlordecone to polar and nonpolar products, and obtained a similar pattern of soluble chlordecone decomposition products with reduced vitamin B_{12} and reduced coenzyme F_{430} isolated from *M. thermophila*.[26] Both cofactors are widely distributed among methanogens[27], which suggests that anaerobic sludges can be used to degrade chlordecone cometabolically.[28] A complementary hypothesis is that anaerobic bacteria can actually obtain energy for growth from the reductive dechlorination of chlordecone. So far there are no indications for the existence of chlordecone respiring organisms[12], but the fact that halorespiring anaerobes exist for a wide variety of aliphatic and aromatic organohalides, including hydrophobic compounds like chlorinated dioxins and PCBs[29], makes such a hypothesis seem reasonable.

A search for chlordecone degrading micro-organisms and other bioremediation tools to clean up chlordecone polluted soils and sediments would benefit from the availability of Gibbs free energy data of chlordecone and its potential dechlorination and degradation products, or more specifically from Gibbs free energy based calculations that show that reductive dechlorination and mineralization of chlordecone are exergonic processes, which would support the hypothesis that organisms exist that perform these reactions and benefit from it. If reductive dechlorination of chlordecone is not exergonic there is no point in searching for organisms that can perform this reaction; similarly there is no point in testing treatment technologies that use reducing conditions; rather one would focus on oxidizing treatments. Presently such data are not available. Polycyclic "cage" molecules of which chlordecone is an example (Figure 1), contain considerable strain energy.[30,31] It is not a priory clear how this affects thermodynamic properties of the chlorinated members of this unique class of compounds, and to what extent redox potentials for the halogenated congeners are different from those of other aliphatic and aromatic organohalogens, which are known to be biodegradable and can serve as electron acceptors in anaerobic environments[22]. We have performed high-level *ab initio* quantum chemical calculations to estimate molar values of $\Delta_f H_m^o$ and $\Delta_f G_m^o$ at 25°C for chlordecone and selected potential dechlorination products, and used these data to estimate the energetics of the degradation and dechlorination of chlordecone under a variety of redox conditions.

MATERIALS AND METHODS

Nomenclature and physical and chemical properties. Chlordecone (MW 490.68) is a tan-white crystalline solid with a melting point of 350 °C. Chlordecone belongs to the bishomocubane family of chemicals.[30] Its IUPAC name is decachloropentacyclo[5.3.0.$0^{2.6}$.$0^{3.9}$.$0^{4.8}$]decan-5-one; its CAS name is 1,1a,3,3a,4,5,5,5a,5b,6-decachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-

one. Both nomenclatures have been used in the literature[32,33] which may create confusion when assigning trivial names for some of the intermediates. In the present work the numbering of the carbons will be according to the IUPAC nomenclature (Figure 1). Registered trade names are Kepone, Curlone, Merex, GC 1189 and ENT16391. Other synonyms include perchloro-1,4-bishomocubanone, decachloroketone, and decachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one.

Quantum chemical calculation methods. *Ab initio* quantum chemical calculations to estimate $\Delta_f H^o_m$ and $\Delta_f G^o_m$ values of chlordecone and selected dechlorination products were performed with the Gaussian 03 software, Revision E.1[34] using the composite G3(MP2)/B3LYP method.[35] This method has a mean absolute deviation (MAD) for $\Delta_f H_m^o$ (g., 298.15 K) in the range of 4-8 kJ/mol.[36] This MAD value corresponds to the "chemical accuracy" (4-8 kJ/mol) which is required for calculated enthalpy values to be both useful in resolving discrepancies between experimental data and for predicting new thermodynamic data[36]. The choice of the method was based on the need to achieve chemical accuracy and also on the computational feasibility of obtaining such accuracy for the specific molecules investigated in this work. The results of our calculations have been checked against the latest proposed experimental $\Delta_f H^o_m$ (g., 298.15 K) values for similar sized (in terms of the numbers of non-H atoms), strained, cage hydrocarbons: cubane (613.0 ±9.5 kJ/mol) and dimethyl 1,4-cubanedicarboxylate (-115.4 ±7.0 kJ/mol)[37]. Our calculated G3MP2B3/B3LYP values of 608.0 and -122.7 kJ/mol, respectively are in good agreement with experimental values. This is important as the "cage" structure of cubane molecules results in strain energy in the carbon skeleton, manifested through long CC bonds and CCC angles that deviate significantly from the tetrahedral 109.5° value.[30] However, the 1,4-bishomocubane structure which provides the backbone of the chlordecone molecule contains two five-member rings and has therefore considerably less strain energy (viz. 306.9 kJ/mol) than cubane itself (695.0 kJ/mol).[31] These values compare favorably with the strain energy for the perchlorinated 1,4-bishomocubane, (783.1 kJ/mol).[31]

The G3(MP2)/B3LYP method yields $\Delta_f G^o_m$ and $\Delta_f H^o_m$ values for the gas phase. For environmental applications data for the aqueous phase are more relevant. We therefore used the DPCM solvation model[38] and G3(MP2)/B3LYP method to simulate water solvent as implemented in the Gaussian software to calculate $\Delta_f G^o_m$ and $\Delta_f H^o_m$ values for the aqueous solution. In the DPCM model, the solvent (in this case water) was represented as a continuous medium with the dielectric constant corresponding to that of water.

Our computational tool was used not because Gaussian software is easy to use, but because it gives good results for the specific set of molecules studied in this work. The use of the tool is also necessary in view of the fact that the experimental methods applied to related cage hydrocarbons[37] (for example the parent cubane) still show discrepancies of 9 kJ/mol in standard enthalpies. This suggests that computational approach for chlordecones is cheaper, faster and more accurate than experimental methods could be at present.

Gibbs free energy values. The G3(MP2)/B3LYP total molecular and atomic energies: H^{mol} , H^{at} , G^{mol} , G^{at} (which included necessary corrections for zero-point-energy,

correction terms for particle motions and for entropy at 298.15K) obtained in the gas phase were converted to $\Delta_f H^o_m$ and $\Delta_f G^o_m$ by using the two expressions below.

$$\Delta_f H^o(g) = H^{mol} - \Sigma(\nu_i H_i^{at}) + \Sigma(\nu_i(\Delta_f H^{at})_i) \;;\; \Delta_f G^o(g) = G^{mol} - \Sigma(\nu_i G_i^{at}) + \Sigma(\nu_i(\Delta_f G^{at})_i)$$

where ν_i is the stoichiometric coefficient of element *i*, $(\Delta_f H^{at})_i$ standard formation enthalpy, $(\Delta_f G^{at})_i$ standard Gibbs free energy of formation of i-th element in the gaseous atomic state. The standard values of thermodynamic functions for carbon, hydrogen, chlorine and oxygen were taken from CODATA database in ref. 39. We have also calculated the appropriate total energies H^{mol}, H^{at}, G^{mol}, G^{at} in the water solvent which allowed us to deduce the solvation energy correction for gas phase data and thus convert $\Delta_f H^o(g)$ and $\Delta_f G^o(g)$ values to $\Delta_f H^o(aq)$ and $\Delta_f G^o(aq)$. The exact expressions for H^{mol}, H^{at}, G^{mol}, G^{at} are given in Gaussian G03 manual.[34]

In aqueous solutions the standard state of all solutes is 1 mol/kg activity, that of water is the pure liquid. Under environmentally relevant conditions the concentrations of substrates and products is not 1 mol/kg. This is considered in $\Delta G'$ values. For a hypothetical reaction aA + bB → cC + dD, $\Delta G'$ values are calculated by using the mass equation

$$\Delta G' = \Delta G^{o\prime} + RT \ln([C]^c[D]^d / [A]^a[B]^b) \qquad (1)$$

The $\Delta G^{o\prime}$ value is obtained from the ΔG^o value by making the appropriate corrections for pH = 7.[40]

Redox Potentials. Redox potentials were calculated with the relationship[40] $E_o' = (-\Delta G^{o\prime}/0.193) - 414$.

Product distribution. The regiospecificity of chlordecone dechlorination was calculated from the $\Delta_f G^o$ values of chlordecone and its potential monohydro substituted dechlorination product according to the equilibrium equation:
chlordecone + H_2 ⇌ monohydrochlordecone + H^+ + Cl^-.
The calculation is based on the premise that $\Delta G_{dechlor} = -RT\ln K_{dechlor}$, where $\Delta G_{dechlor}$ is the change in Gibbs free energy of a reductive dechlorination reaction and $K_{dechlor}$ is the corresponding equilibrium constant, i.e.
$K_{dechlor}$ = [monohydrochlordecone][H^+][Cl^-]/[Chlordecone][H_2].[22] Therefore ($K_{dechlor}$ / [monohydrochlordecone]) = [H^+][Cl^-]/[Chlordecone][H_2]. Thus at a given temperature thermodynamic equilibrium exists between chlordecone and each of its four monohydrochlordecone dechlorination products. Therefore, for each individual monohydrochlordecone the ratio of its concentration over the sum of the concentrations of all four monohydrochlordecones equals the ratio of equilibrium constant with chlordecone over the sum of the equilibrium constants of all four monohydrochlordecones with chlordecone, i.e. for example M_1/M_{total} = $(K_1/(K_1+K_2+K_3+K_4)$ where M_1/M_{total} is the fraction of the products represented by product M_1.[22]

Henry coefficient. The Henry coefficient (H) in units of atm.L/mol was calculated via the formula $\Delta_f G^o_{aq} = \Delta_f G^o_{gas} + RT \ln H$ where R is the universal gas constant (8.314 J/K.mol) and T is temperature in K. The calculations were made for the standard states of 1 M aqueous concentration and 1 atm gas pressure, both at 298.15 K.

RESULTS AND DISCUSSION

The route from chlordecone (perchloro-1,4-bishomocubanone) to its fully dechlorinated product (1,4-bishomocubanone) by sequential dechlorination (removal of 1 Cl at each step without breaking of the carbon structure) encompasses 484 potential intermediates: 92 mesomers plus 196 chirally active compounds (Table 1).

Table 1. Chlordecone and Its Dechlorination Products [a]

dechlorination	-0 Cl	-1 Cl	-2 Cl	-3 Cl	-4 Cl	-5 Cl	-6 Cl	-7 Cl	-8 Cl	-9 Cl	-10 Cl	Σ
meso compounds	1	3	7	12	15	18	15	12	7	3	1	94
enantiomers (x2)	0	1 (2)	9 (18)	24 (48)	38 (76)	52 (104)	38 (76)	24 (48)	9 (18)	1 (2)	0	196 (392)
total without enantiomers	1	4	16	36	53	70	53	36	16	4	1	290
total with enantiomers included	1	5	25	60	91	122	91	60	25	5	1	486

[a] total: 486 congeners, of which 94 are meso compounds and 196 are chiral compounds. Congeners that potentially have a different Gibbs free energy of formation: 290 (94 + 196).

Table SI-1 (Supporting Information) lists all congeners named according to the IUPAC and CAS nomenclatures. In the present manuscript we used a simplified nomenclature based on the chlordecone name using the IUPAC numeration (i.e. the keto group is on carbon 5) in which the position of the hydrogen substituents is indicated (Figure 1). In addition, when one single H is on carbon 10 it may be necessary to specify the relative stereochemistry (*cis* or *trans*) of this H with respect to another hydrogen positioned on the bishomocubane "cage". For instance the trivial name for compound 258 in Table SI-1 (*r*-2,6,*t*-10 trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one, IUPAC nomenclature) will be 1,*r*-3,4,7,8,9,*c*-10-heptahydro-chlordecone which means that the hydrogen on carbon 10 is in the *cis* (*c*-10) position relative to the H on carbon 3 used as reference (*r*-3).

$\Delta_f G^o$ and $\Delta_f H^o$ values for chlordecone and selected dechlorination products in gas and aqueous phases are presented in Table 2. The selection includes the isomers observed when chlordecone is reduced with vitamin B_{12s}.[25] The data for the gas phase are in the format preferred by theoretical chemists because quantum calculations produce the most accurate theoretical results for isolated molecules in the gas phase. The data for the aqueous phase are in the format preferred by environmental chemists and microbiologists. A major advantage of the latter way of presenting $\Delta_f G^o$ data is also that

extrapolation to *in situ* conditions can be easily done by simply substituting the actual concentration for the standard concentration in equation 1. Hereafter we will focus on the data in the aqueous solution. A more extensive Table, which also lists the appropriate strain energies, dipole moments, S^o values and Henry coefficients and includes more compounds, is given in the Supporting Information (Table SI-2).

Table 2. Calculated $\Delta_f G^o$ and $\Delta_f H^o$ Values (kJ/mol) of Chlordecone, Chlordecol and Selected Dechlorinated Congeners in the Gas and the Aqueous Phase [a]

compound	Entry in Table SI-1	$\Delta_f G^o_{gas}$	$\Delta_f H^o_{gas}$	$\Delta_f G^o_{aq}$	$\Delta_f H^o_{aq}$
chlordecone	**1**	**-73.5**	**-225.9**	**-92.0**	**-244.6**
chlordecol	na	-143.5	-332.8	-162.3	-378.0
6-hydrochlordecone	4	-57.8	-205.4	-76.3	-230.0
8-hydrochlordecone*	**5**	**-54.5**	**-201.6**	**-80.5**	**-227.8**
9-hydrochlordecone	3	-54.6	-201.8	-80.1	-227.5
10-hydrochlordecone	**2**	**-52.3**	**-199.2**	**-79.2**	**-226.0**
3,7-dihydrochlordecone*	21	-36.2	-177.9	-68.8	-210.7
cis*-8,10-dihydrochlordecone	**14**	**-31.7**	**-173.3**	**-66.9**	**-209.0**
3,7,10-trihydrochlordecone*	**40**	**-13.2**	**-149.6**	**-53.5**	**-190.2**
8,10,10-trihydrochlordecone*	**34**	**-13.3**	**-150.0**	**-43.7**	**-180.7**
r*-3,7,8,*t*-10-tetrahydrochlordecone	**100**	**20.8**	**-111.6**	**-26.2**	**-158.7**
3,7,10,10-tetrahydrochlordecone*	**77**	**8.8**	**-123.5**	**-27.4**	**-159.9**
3,7,8,10,10-pentahydrochlordecone*	134	43.5	-84.8	2.5	-125.9
2,3,7,8,10,10-hexahydrochlordecone	188	79.1	-45.1	34.9	-89.2
2,3,7,8,9,10,10-heptahydrochlordecone	239	106.4	-14.0	64.0	-56.4
1,2,3,7,8,9,10,10-octahydrochlordecone	276	137.1	20.4	98.9	-17.7
1,2,3,4,6,7,8,9,10-nonahydrochlordecone	286	165.3	52.6	124.2	11.9
1,2,3,6,7,8,9,10,10-nonahydrochlordecone	288	168.3	55.9	131.8	19.6
1,3,4,6,7,8,9,10,10-nonahydrochlordecone*	289	156.2	43.3	119.4	6.8
2,3,4,6,7,8,9,10,10-nonahydrochlordecone	287	162.1	49.0	125.4	12.6
decahydrochlordecone	290	203.8	94.2	171.9	62.5

[a] compounds in bold have been detected in experiments with vitamin B_{12s}[25]; compounds with an asterisk have an enantiomer; na: not applicable

Thermodynamic Data for the Aqueous State. Calculated standard Gibbs free energies of formation ($\Delta_f G^o_{aq}$) of chlordecone and its less chlorinated congeners range between -92.0 and 171.9 kJ/mol for chlordecone and decahydrochlordecone, respectively. $\Delta_f G^o$ decreases with increasing number of chloro substituents (Figure 2). This can be

rationalized by noting that C-H and C-Cl bond enthalpies are 414 and 324 kJ/mol, respectively.[41] Therefore the replacement of C-H by C-Cl bonds leads to the observed effect in $\Delta_f H^o_{aq}$ and $\Delta_f G^o_{aq}$ values. This is also observed for other classes of polycyclic halogenated compounds such as PCBs[42] and chlorodioxins[43] but not for chlorinated aliphatics such as ethanes and ethenes.[44] Considerable variation exists between the thermodynamic values for different congeners with the same degree of chlorination. For the four monochloro congeners for example $\Delta_f G^o_{aq}$ values range between 119.4 kJ/mol for the 2-chloro congener (entry 289 in Table SI-1) and 131.8 kJ/mol for the 4-chloro congener (entry 288 in Table SI-1) respectively. The extent of the variation may depend on the degree of chlorination. It is for instance higher for the dichloro congeners (78.0 to 107.1 kJ/mol) (Table SI-1, Supporting Information), but lower for the monohydrochlordecones (-76.3 to -80.5 kJ/mol). The positions of chlorine substituents (topology) in chlordecone isomers clearly affect $\Delta_f G^o$ values, but the effect is affected by the degree of chlorination of the congeners. It is thus virtually impossible to devise a simple group contribution method to describe the $\Delta_f G^o_{aq}$ of all 486 chlordecone congeners.

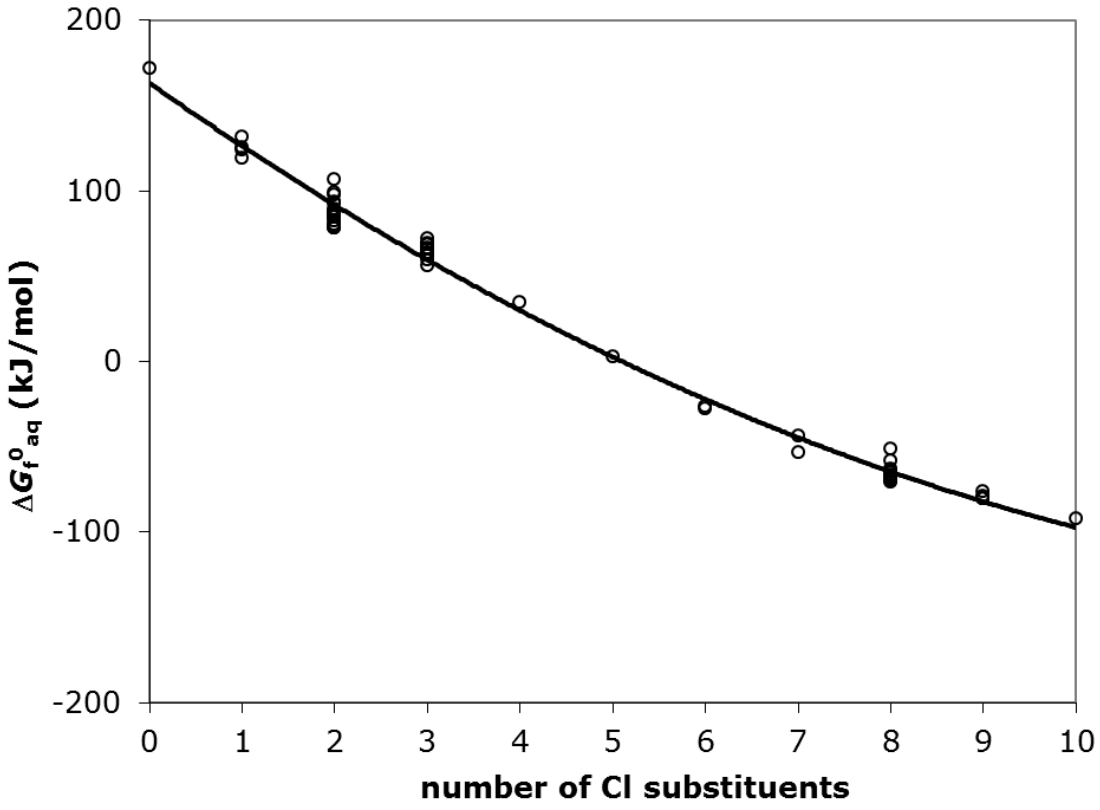

Figure 2. Calculated $\Delta G_f^{\circ}{}_{aq}$ of chlordecone and less halogenated congeners as affected by the degree of chlorination of the molecule (Data Supporting Information - Table SI-2).

The standard Gibbs free energies and enthalpies of formation correlate linearly with strain energy (Figure SI-1, Supporting Information). This can be expected because strain energy is a major (de)stabilizing influence in an individual molecule. We have also noted

that isomers which have chlorine substitution at carbon-10 do not follow this correlation, they represent outliers in Figure SI-1 (Supporting Information). This can be expected because these substituents are attached to relatively strain-free five-member rings. The influence of substitution topology i.e. the location of chlorine atoms on individual molecule's thermodynamic functions does not and cannot be expected to follow simple linear correlations. This is due to the presence of nonlinear quantum mechanical effects (e.g. interatomic steric repulsions, bond dipole repulsions between C-Cl bonds, distortions of CCC bond angles and electron densities in different CC bonds upon vicinal chlorine substitution etc.) which vary with the number and position of chlorine substituents. $\Delta_f G^o_{aq}$ and $\Delta_f H^o_{aq}$ are highly correlated ($r^2 = 0.9993$) as are $\Delta_f G^o_{gas}$ and $\Delta_f H^o_{gas}$ ($r^2 = 0.9996$). $\Delta_f G^o_{aq}$ and $\Delta_f G^o_{gas}$ values correlate less well ($r^2 = 0.9914$), and visual inspection of this correlation suggests that there are systematic effects of substituent pattern on the solvation energy of chlordecone congeners (Figure SI-2; Supporting Information).

Table 3. Calculated Gibbs Free Energy Values and Redox Potentials for the Reductive Dehalogenation of Chlordecone with H_2 as Electron Donor[a]

substrate	product	$\Delta G^{o\prime}$		E_o'
		kJ/reaction	kJ/Cl removed	mV
chlordecone	10-hydrochlordecone	-158.4	-158.4	407
	9-hydrochlordecone	-159.3	-159.3	411
	8-hydrochlordecone	-159.7	-159.7	413
	6-hydrochlordecone	-155.5	-155.5	392
chlordecone	decahydrochlordecone	-1448.1	-144.8	336

[a] Calculated according to the relationship $\Delta G^{o\prime} = \Sigma\, \Delta_f G^o$ (products) – $\Sigma\, \Delta_f G^o$ (reactants) at pH 7, i.e. chlordecone + H_2 → hydrochlordecone + H^+ + Cl^- and chlordecone + 10 H_2 → decahydrochlordecone + 10 H^+ + 10 Cl^-; $\Delta_f G^o$ H^+ at pH 7 = -39.9 kJ/mol (ref 69); $\Delta_f G^o$ Cl^- = -131.3 kJ/mol (ref 69).

Reductive Dechlorination of Chlordecone. Table 3 shows that the reductive dechlorination of chlordecone with H_2 as electron donor is exergonic with reaction free energies under standard conditions (pH = 7) in the range of -145 to -160 kJ/mol of chlorine removed, depending on the dechlorination product formed. This implies that microorganisms can potentially obtain energy for growth from the reductive dechlorination of chlordecone: the $\Delta G^{o'}$ for the dechlorination of chlordecone is well within the range of typical energy yields of -130 to -180 kJ/mol obtained from the dechlorination of a diverse series of chlorinated aliphatic and aromatic compounds that can support growth of the microorganisms involved.[22,45] Per mol of reducing equivalents (H_2) consumed $\Delta G^{o'}$ for the complete dechlorination of chlordecone to decahydrochlordecone is slightly less favorable than for its dechlorination to

monohydrochlordecone, reflecting the fact that the chloro substituents in chlordecone consistently destabilize each other. At redox potentials (E_o') of 336 to 407 mV (Table 3) the redox potential for chlordecone is similar to that of the redox couple NO_3^-/NO_2^- (E_o' = 433 mV). This is substantially higher than the values for sulfate (SO_4^{2-}/SH^-) and bicarbonate (HCO_3^-/CH_4). Based in these values reductive dechlorination of chlordecone is unlikely to occur under aerobic and FeIII reducing conditions.[22,45]

Energy of Dechlorination under *in situ* Conditions. Calculation of ΔG values for chlordecone dechlorination under *in situ* conditions requires information on the actual concentrations of substrates (chlordecone, H_2) and products (H^+, Cl^- and lesser chlorinated chlordecone congeners). We are not aware of any such data sets available in the literature, but lacking those we can make some assumptions. If we assume pH = 7, a chloride concentration of 1 mM (35 mg/L), a hydrogen concentration of 10 Pa (a value typical for methanogenic ecosystems) and concentrations of monohydrochlordecones that are 100 to 1000 fold lower than those of chlordecone (as they are in fish and shellfish)[14] dechlorination of chlordecone under *in situ* conditions in methanogenic environments is 5.7 to 11.4 kJ/mol more favorable than under standard conditions.

Potential Dechlorination Pathway. Based on the ΔG^o values, dechlorination of chlordecone to a mixture of monohydrochlordecone congeners which are in thermodynamic equilibrium with chlordecone consists of 38% 8-hydrochlordecone, 32% 9-hydrochlordecone, 23% 10-hydrochlordecone and 7% 6-hydrochlordecone. Thus a chlordecone dechlorination pathway governed by thermodynamic equilibria will consist of a complex mixture of a wide variety of congeners. A chlordecone dechlorination pathway governed by the rule that the dechlorination pathway solely follows the energetically most favorable steps[46] will result in much simpler mixture of congeners, with only one congener per set of congeners with the same degree of chlorination. For the monohydro and dihydro congeners this would encompass 8-monohydrochlordecone (Table 3) that would later be transformed into 6,7-dihydrochlordecone (Table SI-3, Supporting Information). The differences between the Gibbs free energy of the reactions generating the different possible congeners may in some cases not be higher than the uncertainty in the estimated $\Delta_f G^o_{aq}$ values (e.g. for the monohydrochlordecone the differences range from 0.4 to 4.2 kJ/mol). However, such small differences have been sufficient to explain for instance the formation or absence of formation of dechlorination products of hexachlorobenzene in the environment.[47] Interestingly, 8-monohydro-chlordecone is indeed the only monohydro congener that has been identified as chlordecone alteration product in soil and fish caught in the James River near Hopewell, although it cannot be excluded that this compound occurred as an impurity in the original chlordecone.[48,49] It is also the sole monohydrochlordecone to have been detected after photolysis[32,33] or aerobic microbial attack of chlordecone[24]. Nevertheless, beside the 8-hydro the 10-monohydrochlordecone was also found upon dechlorination with vitamin B_{12S}[25]. The dihydrochlordecones that have been reported to be formed in some of these experiments are the 3,7[24,33] and *cis*-8,10[25] isomers that are only the third and sixth most favorable that can be formed from 8-monohydrochlordecone based on $\Delta G°$ values (Table SI-3). These observations strongly suggest that in these cases dechlorination of chlordecone was subject to kinetic rather than thermodynamic limitations.

Dechlorination versus Alcohol Formation. Chlordecol is the unique identified end product of chlordecone metabolism in man and some other mammals.[50,51] Reduction of the keto group of chlordecone to the corresponding alcohol ($\Delta_f G^o_{aq}$ chlordecol = 162.3 kJ/mol) with hydrogen as electron donor according to the equation chlordecone + H_2 → chlordecol has a $\Delta G^{o'}$ of -70.1 kJ/reaction. Thus reductive dechlorination of chlordecone is energetically more favorable than its reduction to chlordecol. In environments with a limited availability of reducing equivalents (H_2), competition between the two reactions for these equivalents should be in favor of the dechlorination. It is possible however that to maximize recovery of energy certain microorganisms may be able to perform both reactions sequentially or simultaneously. Both ketone and alcohol dechlorinated chlordecone were detected upon reaction with vitamin B_{12S}[25] although the formation of the alcohols as analytical artifacts cannot be ruled out in these experiments.[52]

Fermentation of Chlordecone. From the thermodynamic point of view the high chlorine content of the molecule makes chlordecone less stable: while mineralization of the completely dechlorinated congener according to $C_{10}H_{10}O + 19\ H_2O \rightarrow 10\ CO_2 + 24\ H_2$ is endergonic under standard conditions ($\Delta G^{o'}$ = 390.9 kJ/mol), mineralization of chlordecone according to the equation $C_{10}Cl_{10}O + 19\ H_2O \rightarrow 10\ CO_2 + 10\ H^+ + 10\ Cl^- + 14\ H_2$ ($\Delta G^{o'}$ = -1056.9 kJ/mol) is highly exergonic. This is because carbon-halogen bonds serve as electron acceptors for reducing equivalents generated in the mineralization of the carbon skeleton of the chlordecone molecule. It is tempting to speculate that this opens up the possibilities for organisms to ferment chlordecone into for example acetate and HCl, according to $2\ C_{10}Cl_{10}O + 24\ H_2O \rightarrow 6\ CO_2 + 7\ CH_3COO^- + 27\ H^+ + 20\ Cl^-$ ($\Delta G^{o'}$ = -1389.1 kJ/mol chlordecone). This could be organisms that ferment $C_{10}H_{10}O$ according to $C_{10}H_{10}O + 7\ H_2O + 2\ CO_2 \rightarrow 6\ CH_3COO^- + 6\ H^+$ ($\Delta G^{o'}$ = -178.6 kJ) with relaxed substrate specificity. Such organisms would obtain enough energy for growth from fermentation of the carbon backbone of the molecule.

Dichloroelimination. Dihaloelimination is a known dehalogenation pathway for removal of vicinal halo substituents in halogenated alkanes.[53] Per mole of reducing equivalents used this pathway releases more energy than hydrogenolysis.[22] However, dihaloelimination as a degradation mechanism for chlordecone is unlikely as it would lead to the formation of bridgehead double bonds, which is very improbable due to ring strain and angle strain in particular (violation of Bredt's rule).[54,55]

Chlordecone Mineralization. The Gibbs free energy of a mineralization reaction depends on the type of electron acceptor used, with O_2 being the most favorable and CO_2 the least favorable electron acceptor. Mineralization of chlordecone is exergonic with all the typical electron acceptors found in the environment (Table SI-4, Supporting Information).

Potential degradation pathway under aerobic conditions. With O_2 as reactant the formation of the chlordecone lactone ($\Delta_f G^o_{aq}$ = -239.6 kJ/mol; Figure SI-3) according to the stoichiometry chlordecone + ½ O_2 → chlordecone-lactone is thermodynamically

favorable ($\Delta G^{o'}$ = -147.6 kJ), suggesting that aerobic chlordecone degradation could proceed through a chlordecone lactone pathway. Lactone formation catalyzed by Flavin-dependent-Bayer-Villiger monooxygenases has been observed in other strained cage hydrocarbons such as adamantanone.[56] However, the migrating ability of the alkyl group to form the lactone is decreased if an electron-withdrawing substituent is placed onto the alkyl group.[57] In particular, a significant decrease in reaction rate was observed for α-chloro ketone[57] and as far as we know, Bayer-Villiger monooxygenases have failed to oxidize α-chloro ketone (e.g. ref. 58). Given its structure chlordecone should therefore probably first be partially dehalogenated onto carbon atom 4 or/and 6 before chlordecone lactone formation becomes possible.

Fate of Chlordecone Degradation Products in the Environment. The volatility of chlordecone congeners, as characterized by the Henry coefficient, varies somewhat with the structure (Table SI-2, Supporting Information); there is no correlation between the number of chloro substituents and the volatility of the congener. This can be expected since volatility depends on a molecule's polarity as well as its mass. The solubility of chlordecone congeners as estimated with the EPA SPARC model[59,60] increases with decreasing degree of chlorination (Figure SI-4, Supporting Information). Dechlorination products of chlordecone are thus likely to be more mobile in the environment than their parent compound. This could be a threat since less chlorinated congeners could be more toxic than the parent compound. For instance, vinylchloride, a degradation product of tetra- and trichloroethylene is more harmful than the parent compounds.[61] However comparative toxicity test performed with the few chlordecone congeners available as pure compounds have shown that chlordecone alcohol toxicity ≥ chlordecone > 8-monohydrochlordecone >>> 3,7-dihydrochlordecone which suggests that the toxicity of chlordecone congeners decreases with decreasing degree of chlorination.[50,62] Nevertheless, given the toxicity of the chlordecone itself there is an urgent need for methods that stimulate degradation of this compound in the environment. The present data indicate that there are no thermodynamic constraints which might preclude degradation of chlordecone in the environment and the existence of organisms that obtain energy for growth from the degradation and dechlorination of these compounds.

Steric Constraints and Kinetics. Reductive dechlorination involves the transfer of two electrons to a chlorinated hydrocarbon, and is often kinetically limited by the initial dissociative electron transfer to a C-Cl bond.[63] Whether reduction of a chlorinated hydrocarbon will take place is therefore best evaluated on the basis of one-electron reduction potentials.[53] The present data set the framework for such an analysis: reductive dechlorination of chlordecone is thermodynamically favorable, but whether the reaction will actually proceed at environmentally significant rates and/or at rates which can sustain growth of organisms catalyzing such reactions remains to be determined. Steric factors will also play a role in this, especially in the issue of whether organisms can grow with chlordecone as electron acceptor. In this context it is important to note that (i) similar sized molecules such as PCBs and dioxins can serve as electron acceptors for organohalide respiring bacteria[29] and (ii) compounds of the same substance class are generally dechlorinated faster if they contain a higher number of Cl atoms at the reactive C.[53,64] The size and the highly oxidized carbon skeleton of the chlordecone molecule

should thus be no impediment to the existence of chlordecone respiring bacteria. The xenobiotic nature of the molecule may well be a greater obstacle, but the observation that methanogens[26] and reduced vitamin B_{12} can dechlorinate chlordecone[25] implies that nature already has some of the essential building blocks to evolve such organisms.

Environmental Processes on the French West Indies. Chlordecone fate in the French West Indies can be explained by leaching solely, with no indication of endogenous microorganisms capable of chlordecone degradation.[12] This suggests that bioremediation of chlordecone hotspots will require at least biostimulation, at best bioaugmentation. Reductive dechlorination functions best under reducing conditions, thus biostimulation should rationally encompass stimulation of anaerobic conditions for example by adding sugar cane waste to known chlordecone hotspots. Bioaugmentation would encompass adding chlordecone degraders. Such organisms may well be present in anaerobic niches on the islands, such as sediments and local anaerobic wastewater treatment systems.[65] A viable alternative may also be the use of zero-valent iron or similar *in situ* chemical reduction technologies.[66] All these remediation options will have to face the fact that most of the FWI polluted soils are andosols where chlordecone is strongly bound to the clay-organic matrix which makes it poorly available to chemical or biological agents.[67] This, combined with organic matter stabilization in the fractal pore structure of andosols giving the soils an oxic character and resulting in a lack of reducing equivalents needed for reductive dechlorination possibly explains why natural attenuation of chlordecone has not been observed so far on the FWI.[12,68]

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ASSOCIATED CONTENT

Supporting Information Available. Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names (Table SI-1); Calculated $\Delta_f G^o$, $\Delta_f H^o$, and S^o data for 62 chlordecone congeners plus corresponding Henry constants, strain energy (SE) and dipole (μ) values (Table SI-2); Calculated $\Delta G^{o\prime}$ values for reductive dechlorination of monohydrochlordecone to dihydrochlordecone (Table SI-3);

Change in Gibbs free energy ($\Delta G^{o'}$ in kJ/mol) for mineralization of chlordecone with various electron acceptors (Table SI-4); correlation between calculated $\Delta_f G^o_{gas}$ and strain energy for various classes of chlordecone congeners (Figure SI-1); the correlation between calculated $\Delta G_f^o{}_{aq}$ and $\Delta G_f^o{}_{gas}$ for the 62 chlordecone congeners listed in Table SI-2 (Figure SI-2); the structures of 'chlordecone lactone' plus its calculated $\Delta_f G^o$ and $\Delta_f H^o$ values (Figure SI-3); Estimated solubility of chlordecone congeners versus their degree of chlorination (Figure SI-4). This information is available free of charge via the Internet at http://pubs.acs.org/

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SUPPORTING INFORMATION

Gibbs Free Energy of Formation of Chlordecone and Potential Degradation Products: Implications for Remediation Strategies and Environmental Fate

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CONTENTS:

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

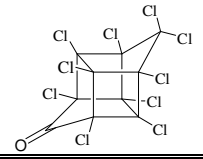
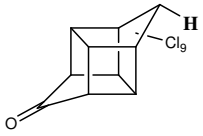
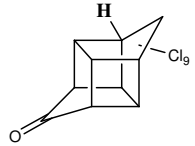
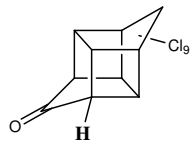
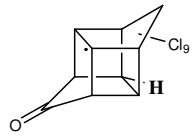
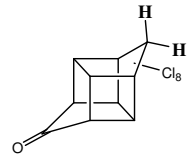
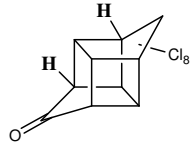
Entry	- nCl	Structure[a]	IUPAC - Name	CAS - Name	Chirality
1	0		decachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,3a,4,5,5,5a,5b,6-decachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
2	1		1,2,3,4,6,7,8,9,10-nonachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,3a,4,5,5a,5b,6-nonachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
3	1		1,2,3,4,6,7,8,10,10-nonachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,3a,4,5,5,5b,6-nonachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
4	1		1,2,3,4,7,8,9,10,10-nonachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3a,4,5,5,5a,5b,6-nonachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
5	1		1,2,3,4,6,7,9,10,10-nonachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,3a,4,5,5,5a,5b-nonachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[c]	*chiral*
6	2		1,2,3,4,6,7,8,9-octachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,3a,4,5a,5b,6-octachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
7	2		1,2,3,6,7,8,10,10-octachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3a,5,5,5a,5b,6-octachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[c]	*meso*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

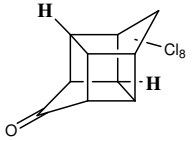
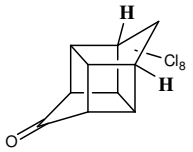
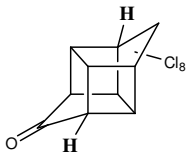
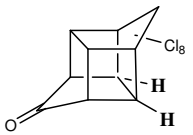
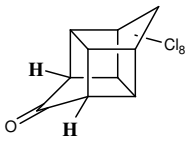
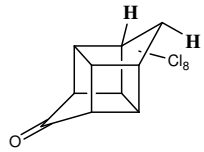
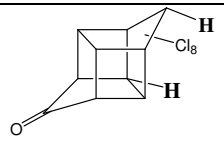
Entry	- nCl	Structure[a]	IUPAC - Name	CAS - Name	Chirality
8	2		1,3,4,6,8,9,10,10-octachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,4,5,5,5a,5b,-octachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[c]	*meso*
9	2		2,3,4,6,7,8,10,10-octachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,3a,5,5,5b,6-octachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
10	2		1,2,3,4,7,8,10,10-octachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3a,4,5,5,5b,6-octachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
11	2		1,2,3,4,6,9,10,10-octachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,4,5,5,5a,6-octachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
12	2		1,2,3,7,8,9,10,10-octachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,3a,4,5,5,5a,5b,6-octachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
13	2		1,2,3,4,6,7,8,10-octachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,3a,4,5,5b,6-octachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
14	2		1,*r*-2,3,4,6,7,9,*c*-10-octachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,3,3a,4,*c*-5,5a,5b-octachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[c]	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

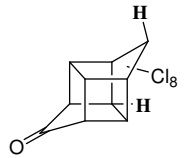
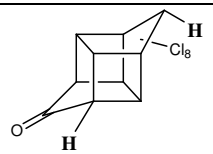
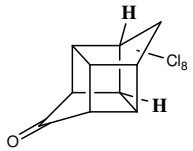
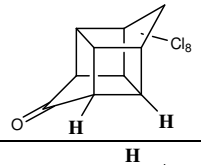
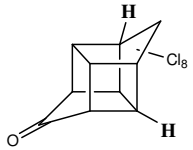
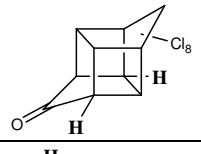
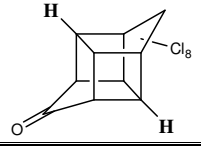
Entry	- nCl	Structure[a]	IUPAC - Name	CAS - Name	Chirality
15	2		1,*r*-2,3,4,6,7,9,*t*-10-octachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,3,3a,4,*c*-5,5a,5b-octachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[c]	*chiral*
16	2		1,2,3,4,7,8,9,10-octachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3a,4,5,5a,5b,6-octachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
17	2		1,2,3,4,6,7,10,10-octachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,3a,5,5,5a,5b-octachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[c]	*chiral*
18	2		1,2,3,4,8,9,10,10-octachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3a,4,5,5,5a,5b-octachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b,c]	*chiral*
19	2		1,2,3,4,6,8,10,10-octachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,3a,4,5,5,5b-octachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b,c]	*chiral*
20	2		1,2,3,4,7,9,10,10-octachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3a,4,5,5,5a,6-octachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
21	2		1,2,4,6,8,9,10,10-octachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,3a,4,5,5,5a-octachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

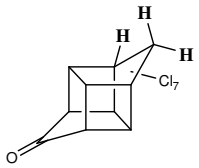
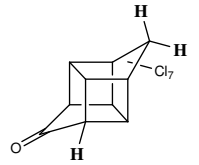
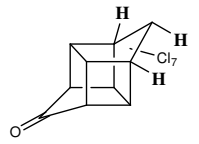
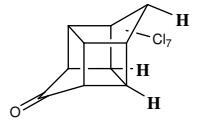
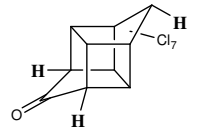
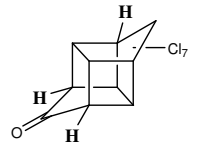
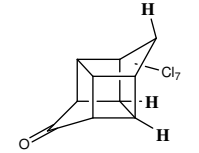
Entry	- nCl	Structure[a]	IUPAC – Name	CAS – Name	Chirality
22	3		1,2,3,4,6,7,8-heptachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1,1a,3,3a,4,5b,6-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
23	3		1,2,3,4,7,8,9-heptachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1,1a,3a,4,5a,5b,6-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
24	3		2,3,4,6,7,8,10-heptachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1,1a,3,3a,5,5b,6-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
25	3		1,*r*-2,3,4,6,9,*c*-10-heptachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,1a,3,4,*c*-5,5a,6-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
26	3		1,2,3,7,8,9,10-heptachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,3a,4,*t*-5,5a,5b,6-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
27	3		1,2,3,7,8,10,10-heptachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1,3a,4,5,5,5b,6-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
28	3		1,*r*-2,3,4,6,9,*t*-10-heptachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,1a,3,4,*t*-5,5a,6-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

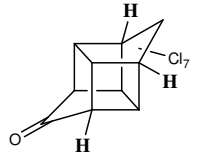
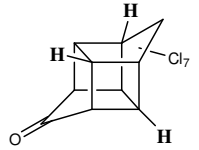
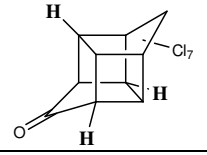
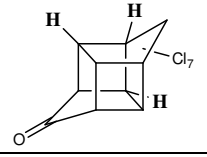
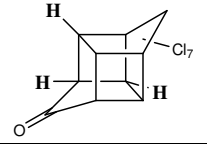
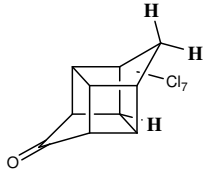
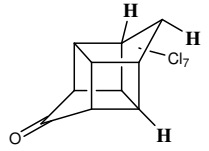
Entry	- nCl	Structure[a]	IUPAC – Name	CAS – Name	Chirality
29	3		2,3,4,7,8,10,10-heptachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3a,5,5,5b,6-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
30	3		1,3,4,6,8,10,10-heptachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,4,5,5,5b-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
31	3		1,2,4,7,9,10,10-heptachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,3,4,5,5,5a,5b-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*meso*
32	3		1,2,4,6,7,10,10-heptachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,5,5,5a,5b-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*meso*
33	3		1,2,6,7,9,10,10-heptachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,4,5,5,5a,5b-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*méso*
34	3		1,2,3,4,6,7,9-heptachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,3a,4,5a,6-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
35	3		1,*r*-2,3,4,6,8,*c*-10-heptachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,3,4,*c*-5,5b,6-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

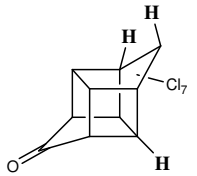
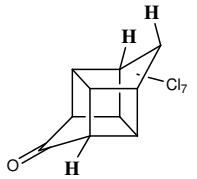
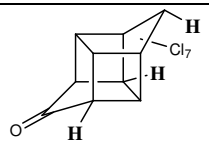
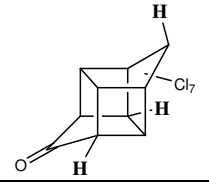
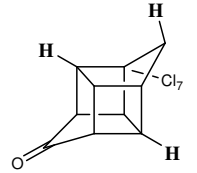
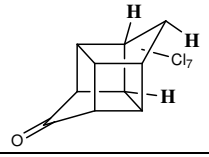
Entry	- nCl	Structure[a]	IUPAC – Name	CAS – Name	Chirality
36	3		1,*r*-2,3,4,6,8,*t*-10-heptachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,3,4,*t*-5,5b,6-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
37	3		1,2,3,4,7,8,10-heptachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3a,4,5,5b,6-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
38	3		1,*r*-2,3,4,7,9,*c*-10-heptachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,3a,4,*c*-5,5a,6-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
39	3		1,*r*-2,3,4,7,9,*t*-10-heptachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,3a,4,*t*-5,5a,6-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
40	3		1,2,4,6,8,9,10-heptachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,3a,4,5,5a-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
41	3		1,*r*-2,3,4,6,7,*c*-10-heptachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,3,3a,4,*c*-5,6-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

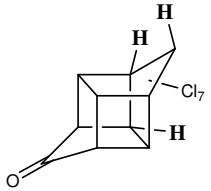
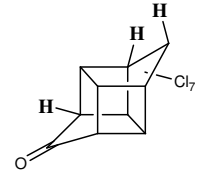
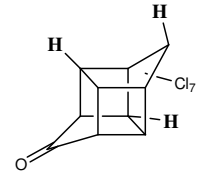
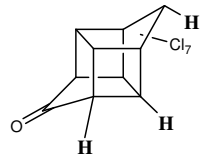
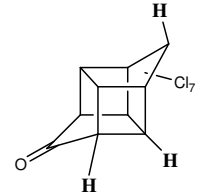
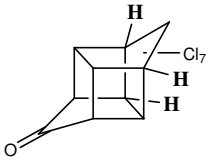
Entry	- nCl	Structure[a]	IUPAC – Name	CAS – Name	Chirality
42	3		1,*r*-2,3,4,6,7,*t*-10-heptachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,3,3a,4,*t*-5,6-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
43	3		1,2,3,6,7,8,10-heptachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3a,5,5a,5b,6-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
44	3		1,2,4,6,7,9,10-heptachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,4,5,5a,5b-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
45	3		1,*r*-2,3,4,8,9,*c*-10-heptachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,4,*c*-5,5a,5b,6-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
46	3		1,*r*-2,3,4,8,9,*t*-10-heptachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,4,*t*-5,5a,5b,6-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
47	3		2,3,4,6,7,10,10-heptachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,3a,5,5,6-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

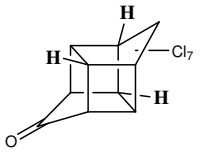
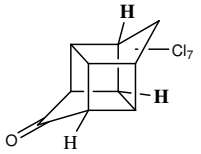
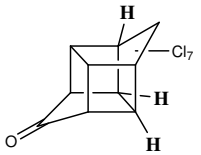
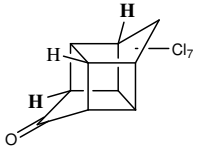
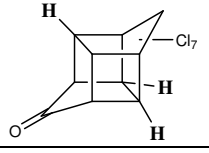
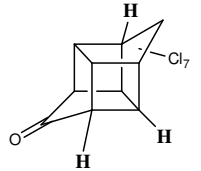
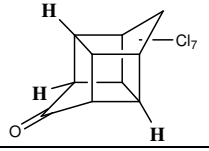
Entry	- nCl	Structure[a]	IUPAC – Name	CAS – Name	Chirality
48	3		1,3,4,6,7,10,10-heptachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,3a,4,5,5-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
49	3		1,2,3,4,7,10,10-heptachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3a,4,5,5,6-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
50	3		1,2,3,4,6,10,10-heptachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,4,5,5,6-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
51	3		1,3,6,7,8,10,10-heptachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,3,3a,4,5,5,5b-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
52	3		1,2,4,6,9,10,10-heptachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,4,5,5,5a-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
53	3		1,2,3,4,8,10,10-heptachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,4,5,5,5b,6-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
54	3		1,2,6,8,9,10,10-heptachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3a,4,5,5,5a-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

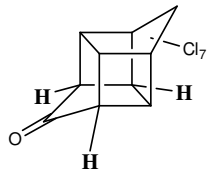
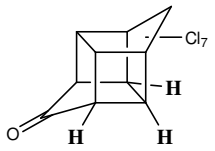
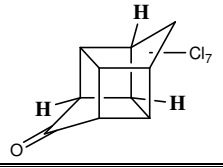
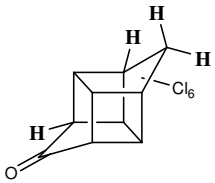
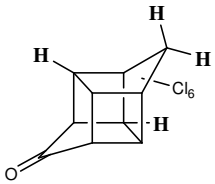
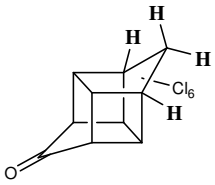
Entry	- nCl	Structure[a]	IUPAC – Name	CAS – Name	Chirality
55	3		1,2,3,7,9,10,10-heptachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,3a,4,5,5,5a,5b-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[c]	*chiral*
56	3		1,2,3,4,9,10,10-heptachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,4,5,5,5a,6-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
57	3		1,2,3,6,7,10,10-heptachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3a,5,5,5a,5b-heptachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[c]	*chiral*
58	4		1,2,3,6,7,8-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3a,5a,5b,6-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*meso*
59	4		1,2,4,6,8,9-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,4,5a,5b-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*meso*
60	4		2,3,4,6,7,8-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,3a,5b,6-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

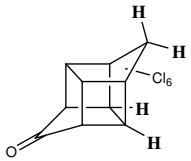
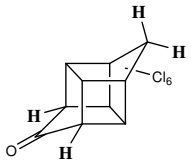
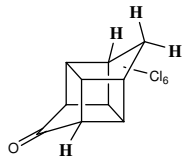
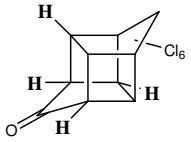
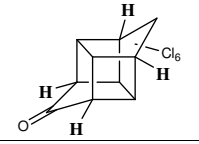
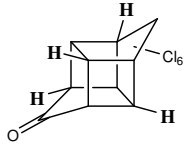
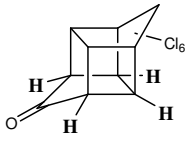
Entry	- nCl	Structure[a]	IUPAC - Name	CAS - Name	Chirality
61	4		1,2,3,4,6,9-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,4,5a,6-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
62	4		1,2,3,7,8,9-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,3a,4,5a,5b,6-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
63	4		1,2,3,4,7,8-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3a,4,5b,6-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
64	4		1,2,7,9,10,10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,4,5,5,5a,5b-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*meso*
65	4		2,3,7,8,10,10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,3a,5,5,5b,6-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
66	4		1,3,6,8,10,10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,3,4,5,5,5b-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
67	4		1,2,3,9,10,10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,4,5,5,5a,6-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

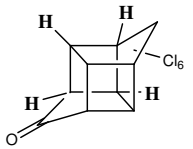
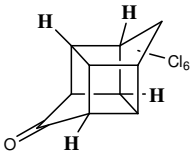
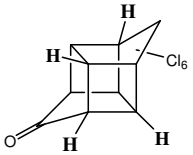
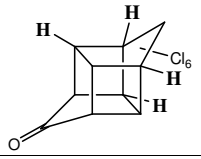
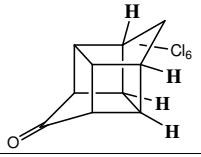
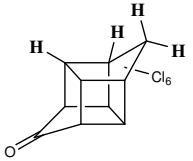
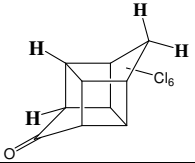
Entry	- nCl	Structure[a]	IUPAC – Name	CAS – Name	Chirality
68	4		1,2,6,7,10,10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,5,5,5a,5b-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*meso*
69	4		1,2,4,7,10,10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,3,5,5,5a,5b-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*meso*
70	4		1,3,4,8,10,10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,4,5,5,5b-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
71	4		2,4,6,7,10,10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,5,5,5b-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*meso*
72	4		2,3,4,6,10,10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,5,5,6-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
73	4		1,2,4,6,7,8-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,3a,5a,5b-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
74	4		1,2,6,7,8,9-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3a,4,5a,5b-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

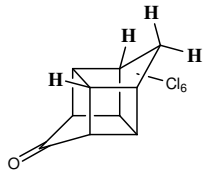
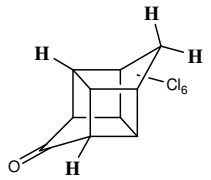
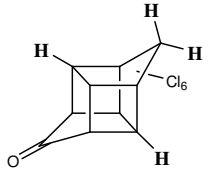
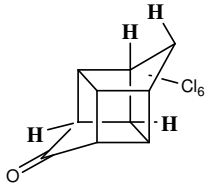
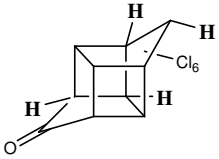
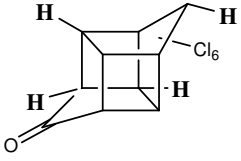
Entry	- nCl	Structure[a]	IUPAC – Name	CAS – Name	Chirality
75	4		1,3,4,6,7,8-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,3a,4,5b-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
76	4		1,2,4,7,8,9-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,3,3a,4,5a,5b-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
77	4		1,2,4,6,8,9-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,3a,4,5a,-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
78	4		1,*r*-2,3,6,7,*t*-10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,*t*-5,5a,5b,6-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
79	4		1,*r*-2,3,6,7,*c*-10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,*c*-5,5a,5b,6-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
80	4		1,2,6,7,9,10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,4,5,5a,5b-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

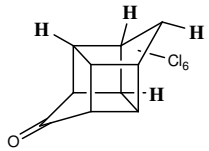
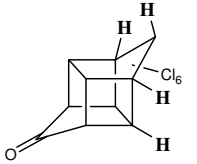
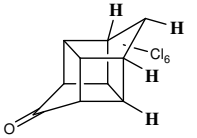
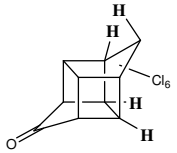
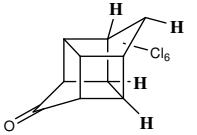
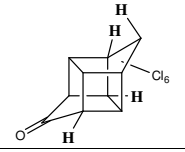
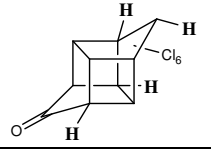
Entry	- nCl	Structure[a]	IUPAC - Name	CAS - Name	Chirality
81	4		1,2,4,6,7,10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,5,5a,5b-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
82	4		*r*-2,3,4,6,8,*t*-10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,3,*t*-5,5b,6-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
83	4		*r*-2,3,4,6,8,*c*-10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,3,*c*-5,5b,6-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
84	4		1,*r*-2,3,4,6,*t*-10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,3,4,*t*-5,6-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
85	4		1,*r*-2,3,4,6,*c*-10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,3,4,*c*-5,6-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
86	4		1,*r*-2,3,4,7,*t*-10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,3a,4,*t*-5,6-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
87	4		1,*r*-2,3,4,7,*c*-10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,3a,4,*c*-5,6-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

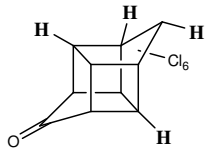
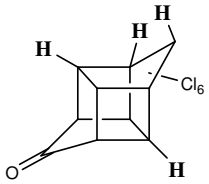
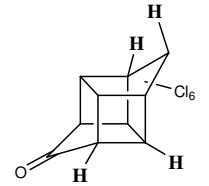
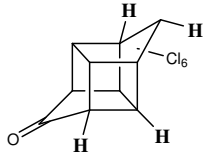
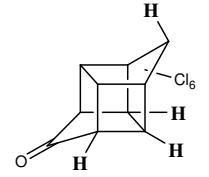
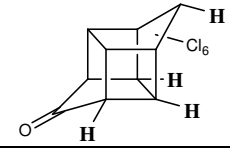
Entry	- nCl	Structure[a]	IUPAC - Name	CAS - Name	Chirality
88	4		1,*r*-2,4,6,8,*c*-10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,3,3a,*c*-5,5a-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
89	4		1,*r*-2,4,6,8,*t*-10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,3,3a,*t*-5,5a-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
90	4		1,*r*-2,3,4,8,*t*-10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,3a,4,*c*-5,5b-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b,c]	*chiral*
91	4		1,*r*-2,3,4,8,*c*-10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,4,*c*-5,5b,6-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
92	4		1,*r*-2,3,4,9,*t*-10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,4,*t*-5,5a,6-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
93	4		1,*r*-2,3,4,9,*c*-10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,4,*c*-5,5a,6-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

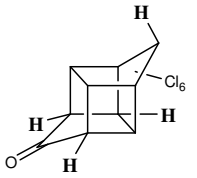
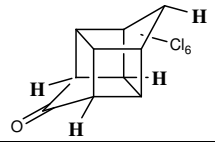
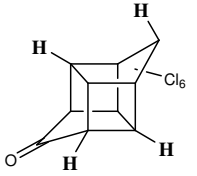
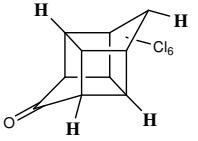
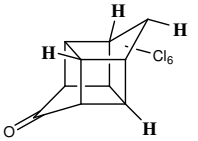
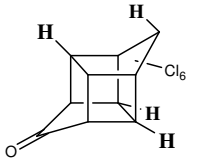
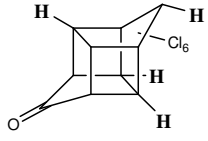
Entry	- nCl	Structure[a]	IUPAC – Name	CAS – Name	Chirality
94	4		1,*r*-2,3,7,9,*t*-10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,3a,4,*c*-5,5a,5b-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[c]	*chiral*
95	4		1,*r*-2,3,7,9,*c*-10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,3a,4,*t*-5,5a,5b-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[c]	*chiral*
96	4		1,*r*-2,4,8,9,*t*-10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,3a,4,*c*-5,5a-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b,c]	*chiral*
97	4		1,*r*-2,4,8,9,*c*-10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,3,3a,4,*t*-5,5a-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b,c]	*chiral*
98	4		1,3,4,6,8,10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,4,5,5b-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
99	4		1,*r*-2,4,6,9,*t*-10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,3,4,*t*-5,5a-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
100	4		1,*r*-2,4,6,9,*c*-10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,3,4,*c*-5,5a-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

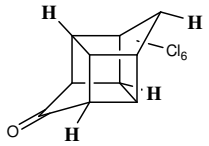
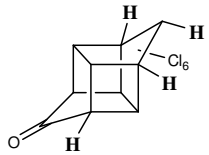
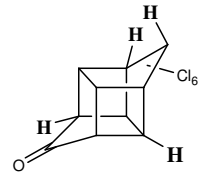
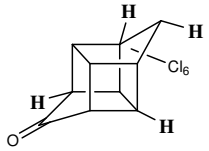
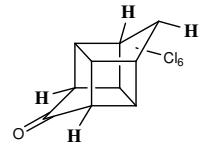
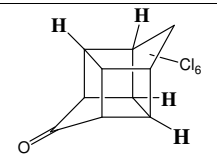
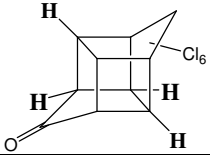
Entry	- nCl	Structure[a]	IUPAC – Name	CAS – Name	Chirality
101	4		1,2,4,7,9,10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,3,4,5,5a,5b-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
102	4		2,3,4,7,8,10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3a,5,5b,6-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
103	4		1,*r*-2,3,6,8,*t*-10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,3a,*t*-5,5a,6-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
104	4		1,*r*-2,3,6,8,*c*-10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,3a,*c*-5,5a,6-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
105	4		1,2,3,7,8,10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,3a,4,5,5b,6-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
106	4		1,2,4,6,10,10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,5,5,5a-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
107	4		1,2,6,9,10,10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,4,5,5,5a,5b-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

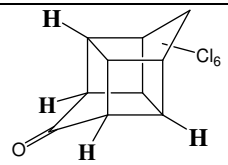
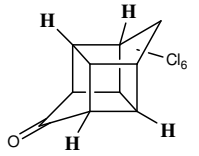
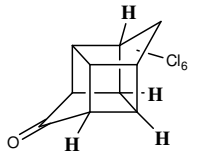
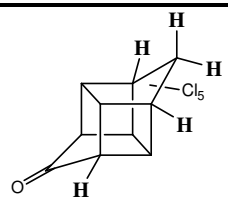
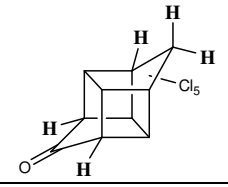
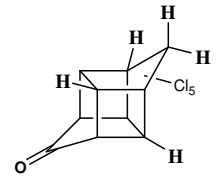
Entry	- nCl	Structure[a]	IUPAC – Name	CAS – Name	Chirality
108	4		1,2,8,9,10,10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,3a,4,5,5,5a-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
109	4		1,2,4,8,10,10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,3,3a,5,5,5a-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
110	4		1,2,3,4,10,10-hexachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,4,5,5,6-hexachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
111	5		2,3,4,7,8-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}] decan-5-one	1,1a,3a,5b,6-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
112	5		1,2,3,7,8-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}] decan-5-one	1,3a,4,5b,6-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
113	5		1,3,4,6,8-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}] decan-5-one	1,1a,3,4,5b-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

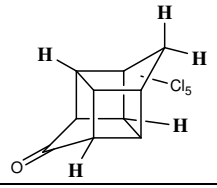
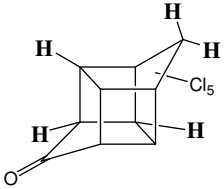
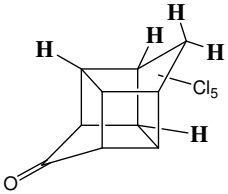
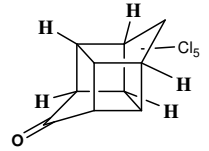
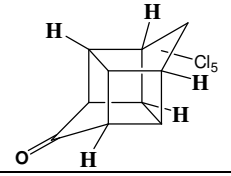
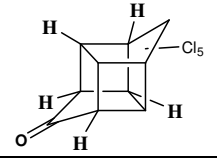
Entry	- nCl	Structure[a]	IUPAC - Name	CAS - Name	Chirality
114	5		1,2,4,7,9-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}] decan-5-one	1,3,4,5a,5b-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*meso*
115	5		1,2,6,7,9-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}] decan-5-one	1,1a,4,5a,5b-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*meso*
116	5		1,2,4,6,7-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}] decan-5-one	1,1a,3,5a,5b-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*meso*
117	5		2,6,7,10,10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}] decan-5-one	1,1a,5,5,5b-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*meso*
118	5		2,4,7,10,10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}] decan-5-one	1,3,5,5,5b-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*meso*
119	5		1,2,7,10,10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}] decan-5-one	1,5,5,5a,5b-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*meso*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

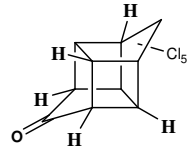
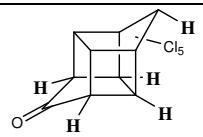
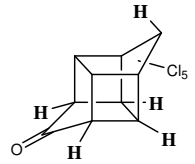
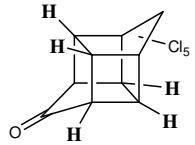
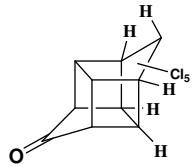
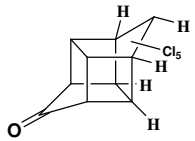
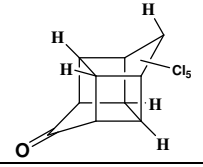
Entry	- nCl	Structure[a]	IUPAC - Name	CAS - Name	Chirality
120	5		1,3,8,10,10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,4,5,5,5b-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
121	5		1,*r*-2,3,9,*c*-10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,4,*c*-5,5a,6-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
122	5		1,*r*-2,3,9,*t*-10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,4,*t*-5,5a,6-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
123	5		1,4,9,10,10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1a,4,5,5,5a-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
124	5		*r*-2,3,4,6,*t*-10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	r-1,1a,3,t-5,6-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
125	5		*r*-2,3,4,6,*c*-10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	r-1,1a,3,c-5,6-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
126	5		1,4,6,9,10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1a,3,4,5,5a-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

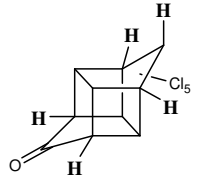
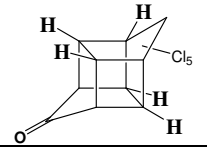
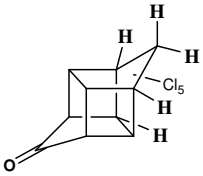
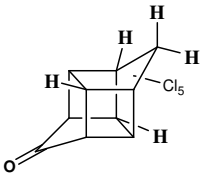
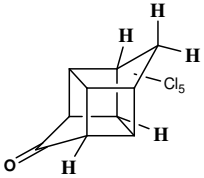
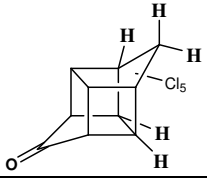
Entry	- nCl	Structure[a]	IUPAC - Name	CAS - Name	Chirality
127	5		2,3,7,8,10-pentachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1,3a,5,5b,6-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
128	5		1,4,6,10,10-pentachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1a,3,4,5,5-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
129	5		2,3,4,6,7-pentachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1,1a,3,3a,5b-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[c]	*chiral*
130	5		1,3,4,6,7-pentachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1,1a,3,3a,4-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
131	5		1,2,3,4,7-pentachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1,1a,3a,4,6-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
132	5		1,2,3,4,6-pentachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1,1a,3,4,6-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

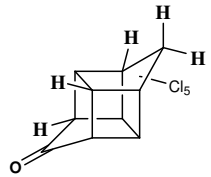
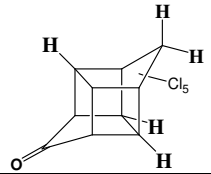
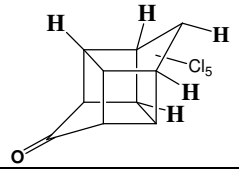
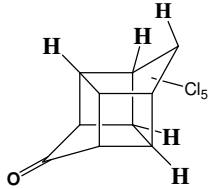
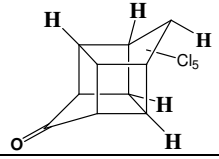
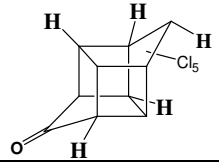
Entry	- nCl	Structure[a]	IUPAC - Name	CAS - Name	Chirality
133	5		1,3,6,7,8-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3a,5a,6-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[c]	*chiral*
134	5		1,2,4,6,9-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,4,5a-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
135	5		2,4,6,7,10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,5,5b-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
136	5		1,*r*-2,4,6,*t*-10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,3,*t*-5,5a-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
137	5		1,*r*-2,4,6,*c*-10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,3,*c*-5,5a-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
138	5		1,2,4,7,10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,3,5,5a,5b-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

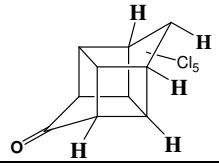
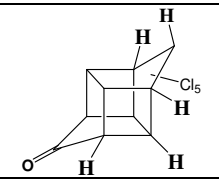
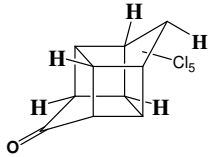
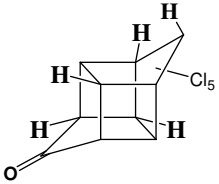
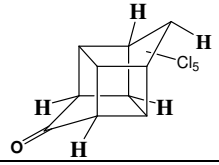
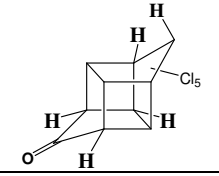
Entry	- nCl	Structure[a]	IUPAC - Name	CAS - Name	Chirality
139	5		r-2,3,4,8,*c*-10-pentachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	r-1,1a,c-5,5b,6-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
140	5		r-2,3,4,8,*t*-10-pentachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	r-1,1a,*t*-5,5b,6-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
141	5		1,*r*-3,6,7,*c*-10-pentachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,1a,3a,*c*-5,5a-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[c]	*chiral*
142	5		1,*r*-3,6,7,*t*-10-pentachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,1a,3a,*t*-5,5a-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[c]	*chiral*
143	5		1,*r*-2,3,7,*c*-10-pentachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,3a,4,*c*-5,6-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
144	5		1,*r*-2,3,7,*t*-10-pentachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,3a,4,*t*-5,6-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

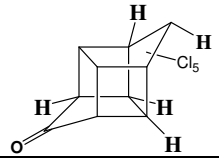
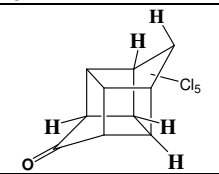
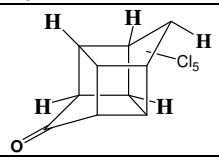
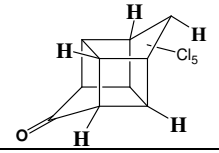
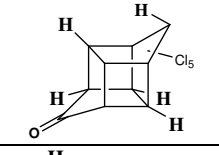
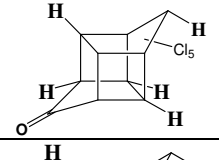
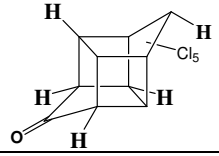
Entry	- nCl	Structure[a]	IUPAC - Name	CAS - Name	Chirality
145	5		1,*r*-2,3,6,*c*-10-pentachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,1a,*c*-5,5a,6-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
146	5		1,*r*-2,3,6,*t*-10-pentachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,1a,*t*-5,5a,6-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
147	5		1,2,6,7,10-pentachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1,1a,5,5a,5b-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
148	5		1,3,4,8,10-pentachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1,1a,4,5,5b-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
149	5		1,*r*-2,6,9,*t*-10-pentachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,1a,4,*t*-5,5a-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
150	5		1,*r*-2,6,9,*c*-10-pentachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,1a,4,*c*-5,5a-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
151	5		1,2,7,9,10-pentachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1,4,5,5a,5b-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

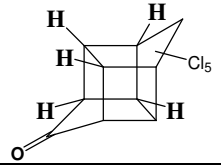
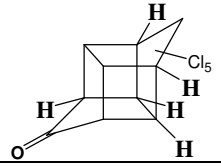
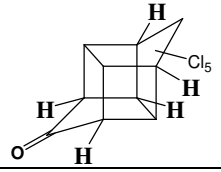
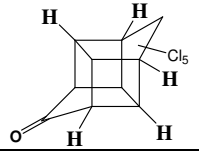
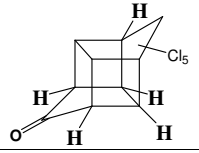
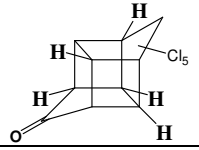
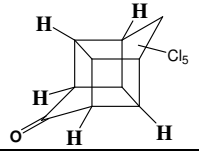
Entry	- nCl	Structure[a]	IUPAC - Name	CAS - Name	Chirality
152	5		1,6,7,10,10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,5,5,5a-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[c]	*chiral*
153	5		2,3,6,10,10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,5,5,6-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
154	5		2,3,7,10,10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,3a,5,5,5b-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[c]	*chiral*
155	5		2,4,8,10,10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,3,3a,5,5-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
156	5		1,2,3,10,10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,4,5,5,6-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
157	5		1,3,6,10,10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,3,4,5,5-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
158	5		1,2,8,10,10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,3a,5,5,5a-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

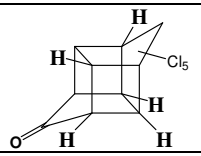
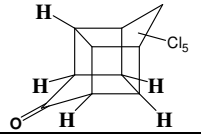
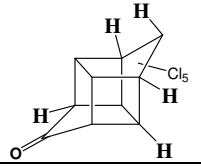
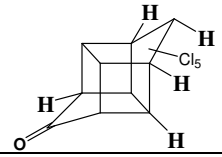
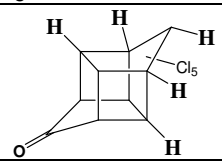
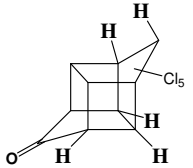
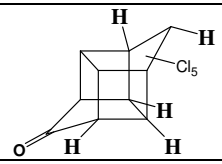
Entry	- nCl	Structure[a]	IUPAC - Name	CAS - Name	Chirality
159	5		1,3,4,10,10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,4,5,5-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
160	5		1,2,9,10,10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,4,5,5,5a-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
161	5		*r*-2,3,6,8,*t*-10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,3a,*t*-5,6-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
162	5		*r*-2,3,6,8,*c*-10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,3a,*c*-5,6-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
163	5		2,4,6,8,10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3,3a,5-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
164	5		1,*r*-2,3,4,*t*-10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,4,*t*-5,6-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
165	5		1,*r*-2,3,4,*c*-10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,4,*c*-5,6-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

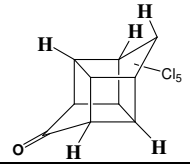
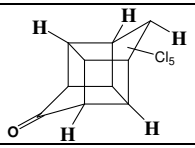
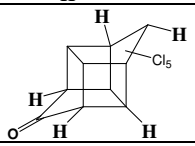
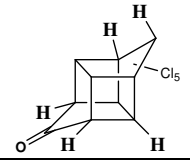
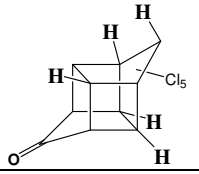
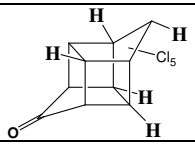
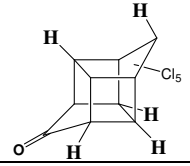
Entry	- nCl	Structure[a]	IUPAC - Name	CAS - Name	Chirality
166	5		1,*r*-2,4,8,*t*-10-pentachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,3,3a,*t*-5,5a-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
167	5		1,*r*-2,4,8,*c*-10-pentachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,3,3a,*c*-5,5a-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
168	5		1,*r*-2,3,8,*c*-10-pentachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,4,*c*-5,5b,6-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
169	5		1,*r*-2,3,8,*t*-10-pentachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,4,*t*-5,5b,6-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
170	5		1,*r*-3,4,6,*t*-10-pentachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,1a,3,4,*t*-5-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
171	5		1,*r*-3,4,6,*c*-10-pentachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,1a,3,4,*c*-5-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta5[cd]pentalen-2-one	*chiral*
172	5		1,*r*-2,4,9,*t*-10-pentachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,3,4,*t*-5,5a-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

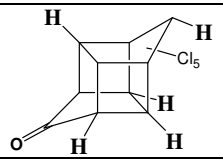
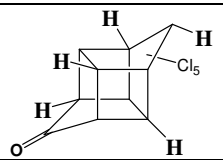
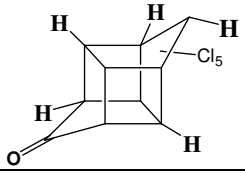
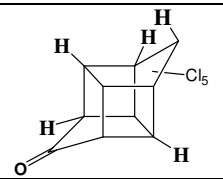
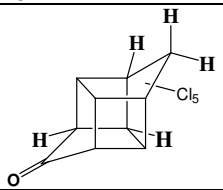
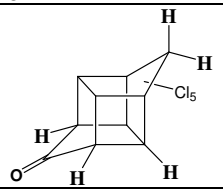
Entry	- nCl	Structure[a]	IUPAC - Name	CAS - Name	Chirality
173	5		1,*r*-2,4,9,*c*-10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,3,4,*c*-5,5a-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
174	5		1,3,6,8,10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,3,4,5,5b-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
175	5		1,*r*-2,6,8,*c*-10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,3a,*c*-5,5a-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
176	5		1,*r*-2,6,8,*t*-10-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,3a,*t*-5,5a-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
177	5		1,2,3,6,7-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,5a,5b,6-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
178	5		1,2,3,8,9-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,4,5a,5b,6-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

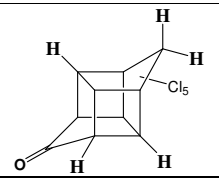
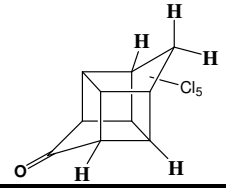
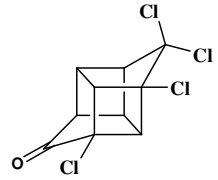
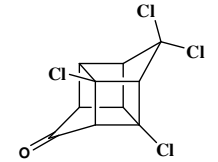
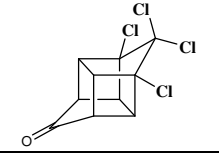
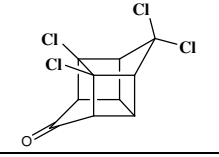
Entry	- nCl	Structure[a]	IUPAC – Name	CAS - Name	Chirality
179	5		1,2,4,8,9-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,3,3a,4,5a-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
180	5		1,2,3,4,8-pentachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,4,5b,6-pentachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
181	6		1,6,10,10-tetrachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1ª,5,5,5ª-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*meso*
182	6		2,7,10,10-tetrachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,5,5,5b-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*meso*
183	6		1,9,10,10-tetrachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	4,5,5,5a-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
184	6		2,3,10,10-tetrachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,5,5,6-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

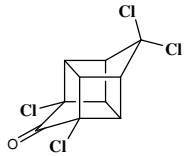
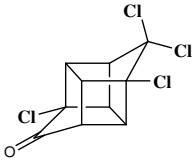
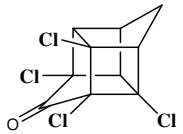
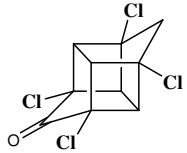
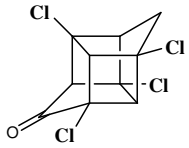
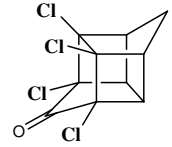
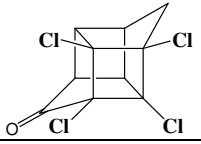
Entry	- nCl	Structure[a]	IUPAC - Name	CAS - Name	Chirality
185	6		4,6,10,10-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1a,3,5,5-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
186	6		1,4,10,10-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1a,4,5,5-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
187	6		2,4,6,7-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1,1a,3,5b-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*meso*
188	6		1,4,6,9-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1a,3,4,5a-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
189	6		1,3,6,8-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1,3,4,5b-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
190	6		2,3,4,6-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1,1a,3,6-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
191	6		1,2,6,7-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1,1a,5a,5b-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[c]	*meso*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

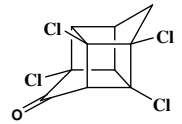
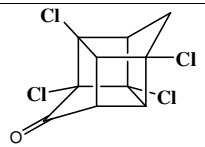
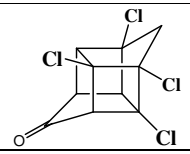
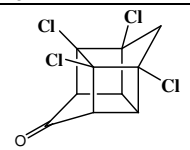
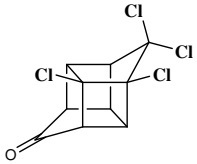
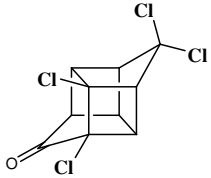
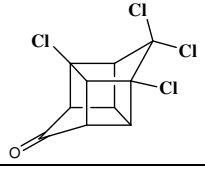
Entry	- nCl	Structure[a]	IUPAC - Name	CAS - Name	Chirality
192	6		1,2,4,7-tetrachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,3,5a,5b-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*meso*
193	6		1,3,4,8-tetrachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,4,5b-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
194	6		1,2,7,9-tetrachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,4,5a,5b-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*meso*
195	6		1,2,3,9-tetrachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,4,5a,6-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
196	6		1,2,10,10-tetrachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,5,5,5a-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
197	6		2,6,10,10-tetrachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,5,5-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
198	6		1,3,10,10-tetrachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,4,5,5-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

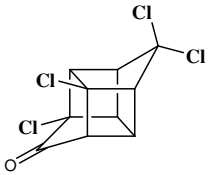
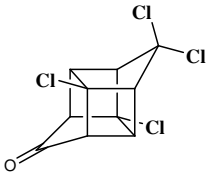
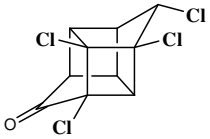
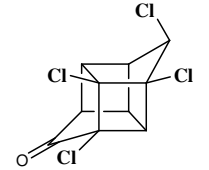
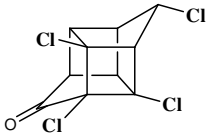
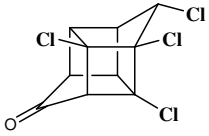
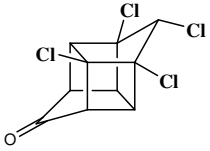
Entry	- nCl	Structure[a]	IUPAC - Name	CAS - Name	Chirality
199	6		2,4,10,10-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1,3,5,5-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
200	6		2,8,10,10-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1,3a,5,5-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
201	6		1,*r*-2,6,*t*-10-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,1a,*t*-5,5a-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
202	6		1,*r*-2,6,*c*-10-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,1a,*c*-5,5a-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
203	6		2,6,7,10-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1,1a,5,5b-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
204	6		1,2,7,10-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1,5,5a,5b-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
205	6		1,*r*-2,9,*t*-10-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,4,*t*-5,5a-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

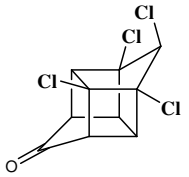
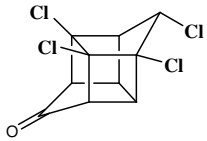
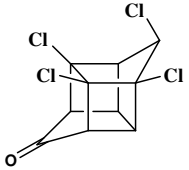
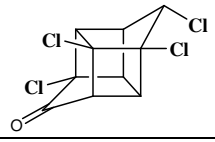
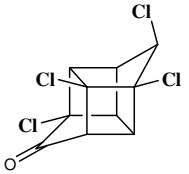
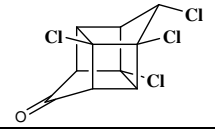
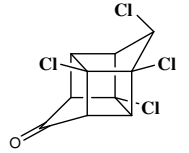
Entry	- nCl	Structure[a]	IUPAC - Name	CAS - Name	Chirality
206	6		1,*r*-2,9,*c*-10-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,4,*c*-5,5a-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
207	6		1,*r*-2,3,*t*-10-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,4,*t*-5,6-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
208	6		1,*r*-2,3,*c*-10-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,4,*c*-5,6-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
209	6		1,*r*-2,4,*t*-10-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,3,*t*-5,5a-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
210	6		1,*r*-2,4,*c*-10-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,3,*c*-5,5a-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
211	6		1,*r*-2,8,*t*-10-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,3a,*t*-5,5a-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
212	6		1,*r*-2,8,*c*-10-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,3a,*c*-5,5a-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

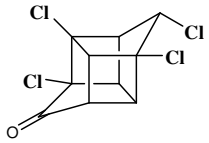
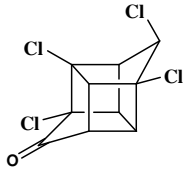
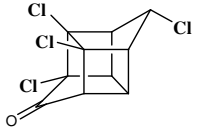
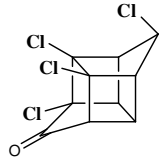
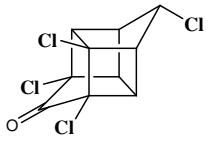
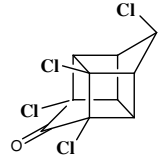
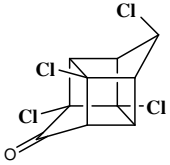
Entry	- nCl	Structure[a]	IUPAC - Name	CAS - Name	Chirality
213	6		1,*r*-3,4,*t*-10-tetrachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,4,*t*-5-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
214	6		1,*r*-3,4,*c*-10-tetrachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,4,*c*-5-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
215	6		*r*-2,3,4,*t*-10-tetrachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,*t*-5,6-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
216	6		*r*-2,3,4,*c*-10-tetrachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,*c*-5,6-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
217	6		*r*-2,4,6,*t*-10-tetrachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,3,*t*-5-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
218	6		*r*-2,4,6,*c*-10-tetrachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,3,*c*-5-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
219	6		*r*-2,4,8,*c*-10-tetrachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,3,3a,*c*-5-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

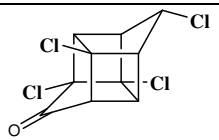
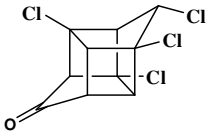
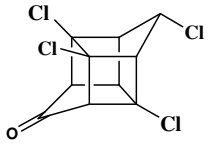
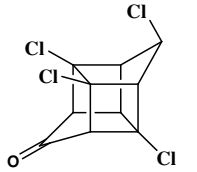
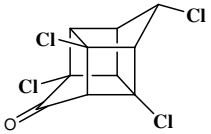
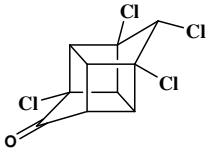
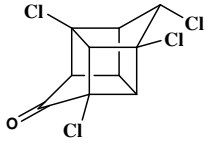
Entry	- nCl	Structure[a]	IUPAC - Name	CAS - Name	Chirality
220	6		*r*-2,4,8,*t*-10-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,3,3a,*t*-5-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
221	6		1,3,8,10-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1,4,5,5b-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
222	6		*r*-2,3,7,*t*-10-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,3a,*c*-5,5b-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[c]	*chiral*
223	6		*r*-2,3,7,*c*-10-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,3a,*t*-5,5b-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[c]	*chiral*
224	6		2,4,7,10-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1,3,5,5b-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
225	6		1,4,9,10-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1a,4,5,5a-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
226	6		1,*r*-3,6,*t*-10-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,3,4,*t*-5-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

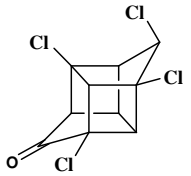
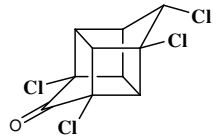
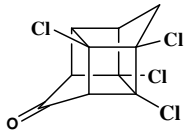
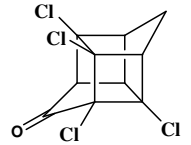
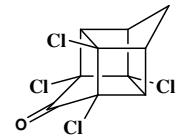
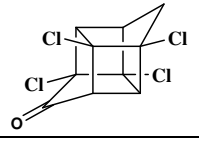
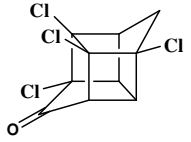
Entry	- nCl	Structure[a]	IUPAC – Name	CAS – Name	Chirality
227	6		1,*r*-3,6,*c*-10-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	*r*-1,3,4,*c*-5-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
228	6		1,4,6,10-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1a,3,4,5-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
229	6		1,2,7,8-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1,3a,5a,5b-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
230	6		2,3,6,7-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1,1a,5b,6-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
231	6		2,4,6,8-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1,1ª,3,3ª-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
232	6		1,2,4,8-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1,3,3ª,5ª-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
233	6		1,2,3,4-tetrachloropentacyclo[5.3.0.$0^{2,6}$.$0^{3,9}$.$0^{4,8}$]decan-5-one	1,1a,4,6-tetrachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

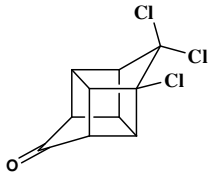
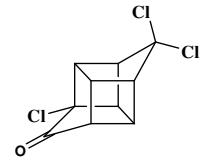
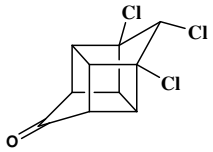
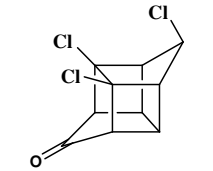
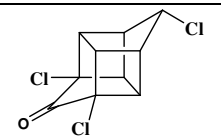
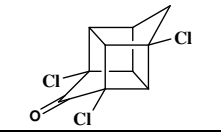
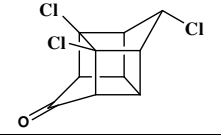
Entry	- nCl	Structure[a]	IUPAC - Name	CAS - Name	Chirality
234	7		1,10,10-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	4,5,5-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
235	7		4,10,10-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1a,5,5-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
236	7		1,9,10-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	4,5,5a-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
237	7		*r*-2,3,*c*-10-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,*c*-5,6-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
238	7		4,6,10-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1a,3,5-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
239	7		1,4,6-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1a,3,4-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
240	7		2,3,10-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,5,6-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

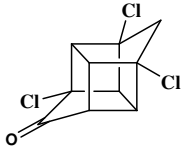
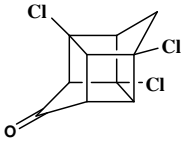
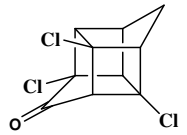
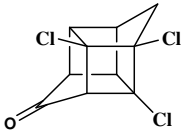
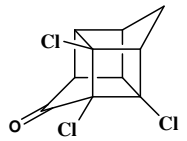
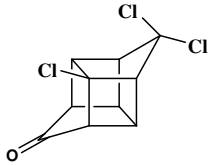
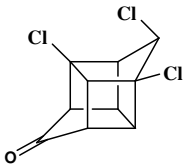
Entry	- nCl	Structure[a]	IUPAC - Name	CAS - Name	Chirality
241	7		1,4,9-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1a,4,5a-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
242	7		1,3,8-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,4,5b-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
243	7		2,4,7-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,3,5b-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*meso*
244	7		1,2,7-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,5a,5b-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*meso*
245	7		2,6,7-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,5b-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*meso*
246	7		2,10,10-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,5,5-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
247	7		1,*r*-3,*c*-10-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,4,*c*-5-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

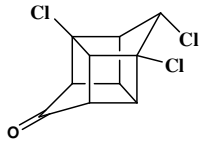
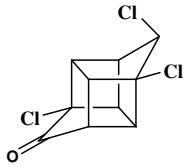
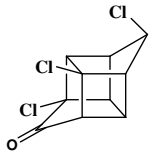
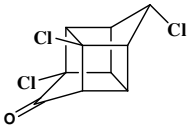
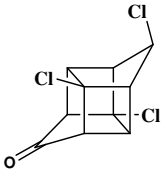
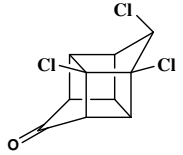
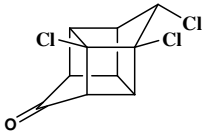
Entry	- nCl	Structure[a]	IUPAC - Name	CAS - Name	Chirality
248	7		1,*r*-3,*t*-10-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,4,*t*-5-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
249	7		1,4,10-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1a,4,5-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
250	7		*r*-2,4,*c*-10-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,3,*c*-5-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
251	7		*r*-2,4,*t*-10-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,3,*t*-5-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
252	7		2,8,10-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,3a,5-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
253	7		1,*r*-2,*c*-10-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,*c*-5,5a-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
254	7		1,*r*-2,*t*-10-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,*t*-5,5a-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

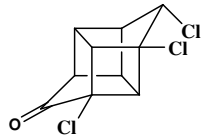
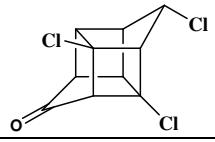
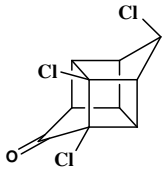
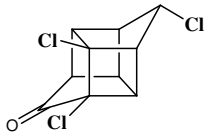
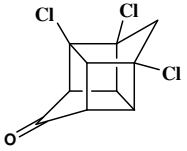
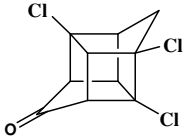
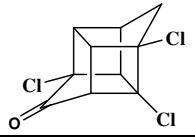
Entry	- nCl	Structure[a]	IUPAC - Name	CAS - Name	Chirality
255	7		1,6,10-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1a,5,5a-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
256	7		2,7,10-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,5,5b-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
257	7		*r*-2,6,*c*-10-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,*c*-5-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
258	7		*r*-2,6,*t*-10-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,1a,*t*-5-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
259	7		1,3,9-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,4,5a-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
260	7		1,3,7-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,3a,4-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
261	7		1,4,7-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1a,3a,4-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

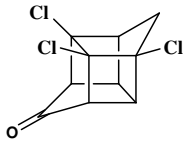
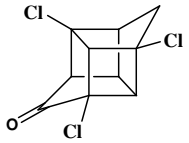
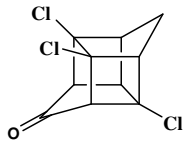
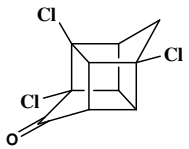
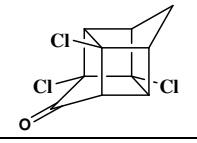
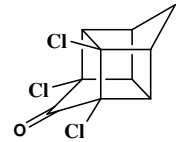
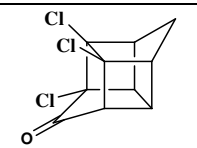
Entry	- nCl	Structure[a]	IUPAC - Name	CAS - Name	Chirality
262	7		1,2,3-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,4,6-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
263	7		1,3,6-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,3,4-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
264	7		2,3,7-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,3a,5b-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[c]	*chiral*
265	7		1,3,4-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,4-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
266	7		2,4,8-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3a-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b,c]	*chiral*
267	7		2,4,6-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,3-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
268	7		2,3,4-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,6-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

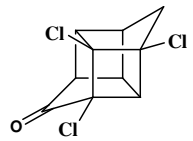
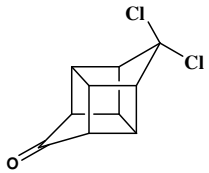
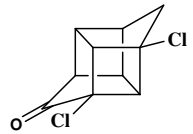
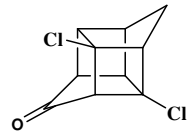
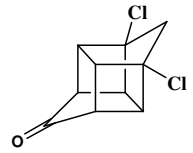
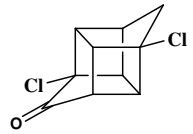
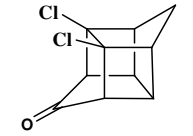
Entry	- nCl	Structure[a]	IUPAC - Name	CAS - Name	Chirality
269	7		1,2,6-trichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a,5a-trichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
270	8		10,10-bichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	5,5-bichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
271	8		1,6-bichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1a,5a-bichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[c]	*meso*
272	8		2,7-bichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,5b-bichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[c]	*meso*
273	8		1,9-bichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	4,5a-bichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
274	8		1,4-bichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1a,4-bichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
275	8		2,3-bichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,6-bichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

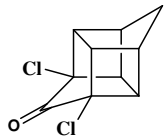
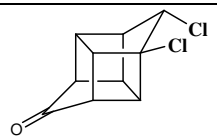
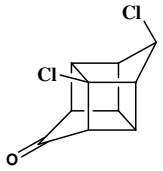
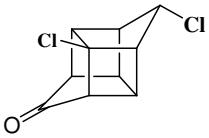
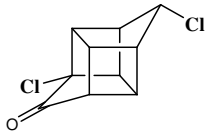
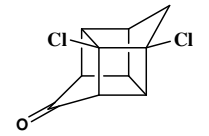
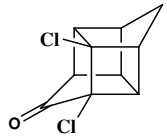
Entry	- nCl	Structure[a]	IUPAC – Name	CAS – Name	Chirality
276	8		4,6-bichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1a,3-bichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
277	8		1,10-bichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	4,5-bichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
278	8		*r*-2,*c*-10-bichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,*c*-5-bichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
279	8		*r*-2,*t*-10-bichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	*r*-1,*t*-5-bichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
280	8		4,10-bichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1a,5-bichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
281	8		1,2-bichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,5a-bichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
282	8		2,6-bichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,1a-bichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

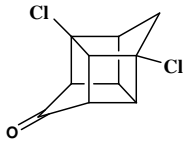
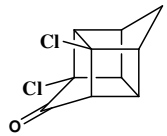
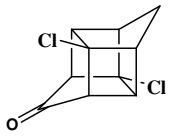
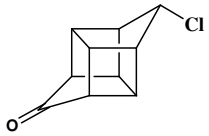
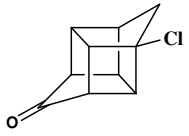
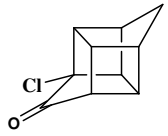
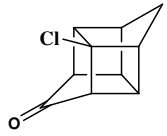
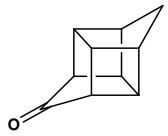
Entry	- nCl	Structure[a]	IUPAC - Name	CAS - Name	Chirality
283	8		1,3-bichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,4-bichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*chiral*
284	8		2,4-bichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,3-bichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
285	8		2,8-bichloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1,3a-bichlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*
286	9		10-monochloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	5-monochlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
287	9		1-monochloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	4-monochlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
288	9		4-monochloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1a-monochlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*
289	9		2-monochloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	1-monochlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[b]	*chiral*

Table SI-1 Structures of all chlordecone potential dechlorinated congeners and their IUPAC and CAS names

Entry	- nCl	Structure[a]	IUPAC - Name	CAS - Name	Chirality
290	10		pentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decan-5-one	octahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one	*meso*

a - The structures represented in the Table corresponds to the IUPAC numerotation.
b - The CAS name corresponds to the enantiomer of the IUPAC structure represented in the same line
c - The CAS name corresponds to a C_2 rotation (180°) around the carbonyl bound, of the IUPAC structure represented in the same line.

Table SI-2. Calculated $\Delta_f G^o$, $\Delta_f H^o$, and S^o data for 62 chlordecone congeners plus corresponding Henry constants, strain energy (SE) and dipole (μ) values[a]

Compound	Entry in Table SI-1	$\Delta_f H^o_{gas}$ (kJ/mol)	S^o_{gas} (J/mol.K)	$\Delta_f G^o_{gas}$ (kJ/mol)	$\Delta_f H^o_{aqueous}$ (kJ/mol)	$S^o_{aqueous}$ (J/mol.K)	$\Delta_f G^o_{aqueous}$ (kJ/mol)	SE (kJ/mol)	μ D	*H* (atm.L/mol)
chlordecone	1	-225.9	764	-73.5	-244.6	764	-92.0	483.7	1.78	5.76E-04
chlordecol	NA	-332.8	771	-143.5	-378.0	682	-162.3	433.4	2.24	5.10E-04
10-monohydrochlordecone	2	-199.2	736	-52.3	-226.0	737	-79.2	478.7	2.44	1.95E-05
9-monohydrochlordecone	3	-201.8	735	-54.6	-227.5	735	-80.1	455.7	2.37	3.42E-05
8-monohydrochlordecone*	5	-201.6	736	-54.5	-227.8	735	-80.5	455.9	1.97	2.80E-05
6-monohydrochlordecone	4	-205.4	734	-57.8	-230.0	714	-76.3	452.1	1.68	5.66E-04
10,10-dihydrochlordecone	6	-176.4	707	-34.5	-200.3	706	-58.1	458.4	3.45	7.36E-05
9,10-dihydrochlordecone*	13	-174.7	707	-32.9	-207.4	706	-65.2	451.0	3.15	2.20E-06
cis-8,10-dihydrochlordecone*	14	-173.3	708	-31.7	-209.0	706	-66.9	452.4	3.00	6.85E-07
trans-8,10-dihydrochlordecone*	15	-174.8	708	-33.2	-207.9	707	-66.1	451.0	2.28	1.73E-06
8,9-dihydrochlordecone*	17	-178.1	706	-35.9	-210.2	706	-67.9	427.3	2.85	2.49E-06
7,9-dihydrochlordecone*	19	-177.1	710	-36.0	-211.1	692	-64.6	428.3	2.39	9.76E-06
7,8-dihydrochlordecone	11	-171.3	705	-28.8	-205.7	705	-63.1	434.1	2.71	1.00E-06
6,10-dihydrochlordecone*	16	-178.7	706	-36.6	-211.5	705	-69.1	447.0	2.30	2.03E-06
6,9-dihydrochlordecone	10	-180.7	705	-38.3	-211.6	705	-69.1	424.7	1.67	4.04E-06
6,8-dihydrochlordecone*	20	-180.7	706	-38.4	-212.1	705	-69.7	424.7	1.68	3.30E-06
6,7-dihydrochlordecone*	18	-181.4	704	-38.7	-213.2	704	-70.4	424.0	2.30	2.81E-06
4,9-dihydrochlordecone	7	-177.6	705	-35.1	-210.9	704	-68.2	427.8	2.76	1.60E-06
4,6-dihydrochlordecone	12	-182.6	704	-39.7	-211.9	704	-69.0	422.9	0.72	7.39E-06
3,8-dihydrochlordecone	8	-173.2	707	-31.3	-193.4	707	-51.4	432.3	1.86	3.02E-04
3,7-dihydrochlordecone*	21	-177.9	708	-36.2	-210.7	707	-68.8	427.6	1.69	1.95E-06
1,9-dihydrochlordecone	9	-175.5	706	-33.4	-206.7	705	-64.3	429.9	2.61	3.88E-06
8,10,10-trihydrochlordecone*	34	-150.0	678	-13.3	-180.7	677	-43.7	432.7	3.65	4.74E-06
3,7,10-trihydrochlordecone*	40	-149.6	679	-13.2	-190.2	678	-53.5	424.1	2.47	8.75E-08
3,7,10,10-tetrahydrochlordecone*	77	-123.5	647	8.8	-159.9	646	-27.4	407.1	3.50	4.57E-07
r-3,7,8,t-10-tetrahydrochlordecone*	100	-111.6	647	20.8	-158.7	646	-26.2	410.0	3.43	5.99E-09
3,7,8,10,10-pentahydrochlordecone*	134	-84.8	614	43.5	-125.9	614	2.5	393.8	3.89	6.60E-08
2,3,7,8,10,10-hexahydrochlordecone	188	-45.1	582	79.1	-89.2	582	34.9	381.3	3.57	1.82E-08
3,4,7,8,9,10,10-heptahydrochlordecone*	269	-23.9	546	97.0	-52.4	546	68.5	277.8	6.09	1.04E-05
r-3,4,6,7,8,9,c-10-heptahydrochlordecone*	254	-31.5	548	88.8	-56.4	549	63.7	333.8	3.07	4.07E-05
2,6,7,8,9,10,10-heptahydrochlordecone*	265	-30.2	548	90.2	-54.6	548	65.8	271.5	4.23	5.40E-05
r-2,4,6,7,8,9,c-10-heptahydrochlordecone*	248	-33.0	550	86.9	-56.7	550	63.1	332.4	1.78	6.65E-05
2,3,7,8,9,10,10-heptahydrochlordecone	239	-14.0	548	106.4	-56.4	548	64.0	360.4	4.96	3.75E-08
1,6,7,8,9,10,10-heptahydrochlordecone*	268	-26.7	546	94.3	-52.9	545	68.4	274.9	6.09	2.91E-05
1,3,7,8,9,10,10-heptahydrochlordecone*	267	-23.7	548	96.8	-48.3	548	72.1	278.0	5.85	4.74E-05
1,3,6,7,9,10,10-heptahydrochlordecone*	266	-36.5	548	83.8	-60.6	549	59.7	265.2	5.00	6.02E-05
1,3,4,8,9,10,10-heptahydrochlordecone	245	-30.4	547	90.4	-54.8	547	66.0	271.3	5.78	5.22E-05
1,3,4,6,8,9,10-Heptahydrochlordecone*	256	-32.3	551	87.4	-57.1	551	62.4	333.0	3.26	4.25E-05
1,3,4,6,7,9,10-heptahydrochlordecone*	252	-37.1	551	82.5	-63.0	551	56.5	328.2	2.62	2.77E-05
1,3,4,6,7,8,9-heptahydrochlordecone*	246	-27.6	547	93.1	-51.2	548	69.2	337.8	2.37	6.55E-05
1,r-3,4,7,8,9,c-10-heptahydrochlordecone*	258	-27.7	549	92.3	-53.5	550	66.5	337.6	3.97	2.97E-05
3,4,6,7,8,9,10,10-octahydrochlordecone*	281	3.5	514	120.4	-36.0	515	80.6	325.8	4.72	1.08E-07
2,4,6,7,8,9,10,10-octahydrochlordecone*	283	1.5	515	117.9	-37.5	516	78.7	323.8	3.87	1.35E-07
2,3,6,7,8,9,10,10-octahydrochlordecone	274	13.7	514	130.4	-9.5	515	107.1	336.0	3.88	8.31E-05
2,3,4,7,8,9,10,10-octahydrochlordecone	271	19.3	514	136.2	-23.4	514	93.4	341.6	5.58	3.17E-08
2,3,4,6,7,8,10,10-octahydrochlordecone	273	7.3	515	123.9	-31.2	515	85.2	329.6	2.06	1.67E-07
2,3,4,6,7,8,9,10-octahydrochlordecone*	277	12.3	515	128.8	-31.8	516	84.4	325.6	2.82	1.70E-08
1,4,6,7,8,9,10,10-octahydrochlordecone	275	5.7	513	122.7	-34.4	514	82.3	328.0	5.51	8.51E-08
1,3,6,7,8,9,10,10-octahydrochlordecone*	284	8.1	515	124.7	-30.8	515	85.6	330.4	5.40	1.42E-07
1,3,4,6,8,9,10,10-octahydrochlordecone	272	0.2	515	116.6	-37.1	516	79.1	322.5	4.54	2.69E-07
1,r-3,4,6,7,8,9,t-10-octahydrochlordecone*	278	8.9	516	125.1	-37.9	517	78.1	322.2	4.28	5.80E-09
1,r-3,4,6,7,8,9,c-10-octahydrochlordecone*	279	4.8	517	120.8	-18.1	517	97.7	318.0	2.44	9.00E-05
1,3,4,7,8,9,10,10-octahydrochlordecone*	282	9.6	514	126.5	-29.7	514	87.0	331.9	5.91	1.21E-07
1,3,4,6,7,9,10,10-octahydrochlordecone*	285	-4.8	515	111.6	-26.6	516	89.6	317.6	4.04	1.40E-04
1,2,3,7,8,9,10,10-octahydrochlordecone	276	20.4	514	137.1	-17.7	515	98.9	342.7	5.70	2.04E-07
1,2,3,6,7,8,9,10-octahydrochlordecone*	280	16.5	516	132.8	-27.9	517	88.2	329.8	3.96	1.53E-08
1,2,3,4,6,7,8,9-octahydrochlordecone	270	15.7	513	132.7	-24.0	514	92.7	308.7	1.01	1.00E-07
2,3,4,6,7,8,9,10,10-nonahydrochlordecone	287	49.0	480	162.1	12.6	481	125.4	319.3	3.82	3.71E-07
1,3,4,6,7,8,9,10,10-nonahydrochlordecone*	289	43.3	481	156.2	6.8	482	119.4	313.5	4.79	3.59E-07
1,2,3,6,7,8,9,10,10-nonahydrochlordecone	288	55.9	483	168.3	19.6	483	131.8	289.8	5.42	4.05E-07
1,2,3,4,6,7,8,9,10-nonahydrochlordecone	286	52.6	482	165.3	11.9	483	124.2	313.8	2.70	6.44E-08
decahydrochlordecone	290	94.2	446	203.8	62.5	446	171.9	312.3	4.18	2.59E-06

[a]Compounds with an asterisk have an enantiomer.

Table SI-3. Calculated $\Delta G°'$ values for reductive dechlorination of monohydrochlordecone to dihydrochlordecone [a]

Reactant	Entry in Tab SI-1	Dechlorination product	Entry in Tab SI-1	$\Delta G°'$ kJ/mol
10-monohydrochlordecone	2	**6,10-dihydrochlordecone***	**16**	**-161.1**
		cis-8,10-dihydrochlordecone*	14	-158.9
		trans-8,10-dihydrochlodecone*	15	-158.1
		9,10-dihydrochlordecone*	13	-157.2
		10,10-dihydrochlordecone	6	-150.1
9-monohydrochlordecone	3	**6,9-dihydrochlordecone**	**10**	**-160.2**
		4,9-dihydrochlordecone	7	-159.3
		8,9-dihydrochlordecone*	17	-159.0
		9,10-dihydrochlordecone*	13	-156.3
		7,9-dihydrochlordecone*	19	-155.7
		1,9-dihydrochlordecone	9	-155.4
8-monohydrochlordecone*	5	**6,7-dihydrochlordecone***	**18**	**-161.1**
		6,8-dihydrochlordecone*	20	-160.4
		3,7-dihydrochlordecone*	21	-159.5
		8,9-dihydrochlordecone*	17	-158.6
		cis-8,10-dihydrochlordecone*	14	-157.6
		trans-8,10-dihydrochlodecone*	15	-156.8
		7,9-dihydrochlordecone*	19	-155.3
		7,8-dihydrochlordecone	11	-153.7
		3,8-dihydrochlordecone	8	-142.1
6-monohydrochlordecone	4	**6,7-dihydrochlordecone***	**18**	**-165.3**
		6,8-dihydrochlordecone*	20	-164.6
		6,10-dihydrochlordecone*	16	-164.0
		6,9-dihydrochlordecone	10	-164.0
		4,6-dihydrochlordecone	12	-163.9
		4,9-dihydrochlordecone	7	-163.1

[a] Calculated according to the relationship: hydrochlordecone + H_2 → dihydrochlordecone + H^+ + Cl^- ; $\Delta_f G^o$ H^+ at pH 7 = -39.9 kJ/mol; $\Delta_f G^o$ Cl^- = -131.3 kJ/mol.[69] The most favorable reactions are indicated in red.

* Compounds with an asterisk have an enantiomer that can be produced from the monohydrochlodecone indicated. The dihydro chiral compounds obtained from 8-monohydrochlordecone will be in racemic mixture if the starting compound is racemic, otherwise, only one of the enantiomers will be generated.

Table SI-4. Change in Gibbs free energy ($\Delta G^{o'}$ in kJ/mol) for mineralization of chlordecone with various electron acceptors[a]

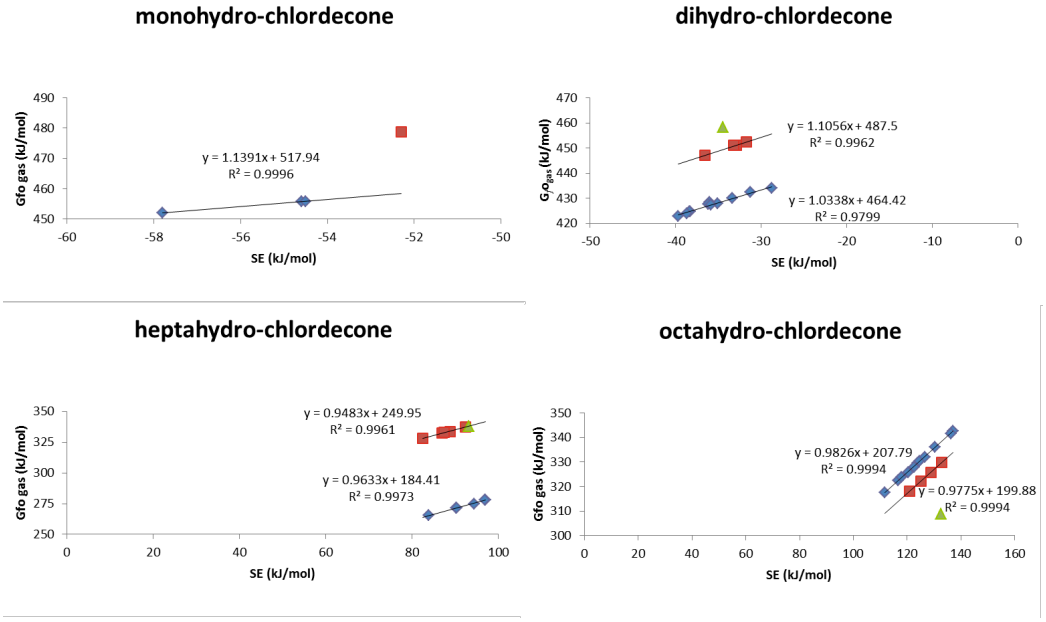
reactants	products	$\Delta G^{o'}$
$C_{10}Cl_{10}O + 5\ H_2O + 7\ O_2$	$\rightarrow 10\ CO_2 + 10\ H^+ + 10\ Cl^-$	-4377
$C_{10}Cl_{10}O + 19\ H_2O + 28\ Fe^{3+}$	$\rightarrow 10\ CO_2 + 38\ H^+ + 10\ Cl^- + 28\ Fe^{2+}$	-4252
$C_{10}Cl_{10}O + 5\ H_2O + 14\ NO_3^-$	$\rightarrow 10\ CO_2 + 10\ H^+ + 10\ Cl^- + 14\ NO_2^-$	-3339
$5\ C_{10}Cl_{10}O + 11\ H_2O + 28\ NO_3^-$	$\rightarrow 50\ CO_2 + 22\ H^+ + 50\ Cl^- + 14\ N_2$	-4195
$2\ C_{10}Cl_{10}O + 7\ SO_4^{2-} + 10\ H_2O$	$\rightarrow 20\ CO_2 + 13\ H^+ + 20\ Cl^- + 7\ HS^-$	-1589
$2\ C_{10}Cl_{10}O + 24\ H_2O$	$\rightarrow 13\ CO_2 + 20\ H^+ + 20\ Cl^- + 7\ CH_4$	-1514

[a] Gibbs free energy of formation data for inorganic compounds were taken from Stumm and Morgan (1996).

Literature Cited

Stumm, W.; Morgan, J. J. Aquatic Chemistry, 3rd edition. Wiley-Interscience, New York, 1996.

Figure SI-1. Correlation between calculated $\Delta_f G^o_{gas}$ and strain energy for various classes of chlordecone congeners



green triangles	congeners containing chlorosubstituents at both 10-positions
red squares	congeners containing a chlorosubstituent at one of the 10-positions
blue diamonds	congeners without chlorosubstituents at the 10-positions

Figure SI-2. Correlation between calculated $\Delta_f G^o_{aq}$ and $\Delta_f G^o_{gas}$ for the 62 chlordecone congeners listed in Table SI-2

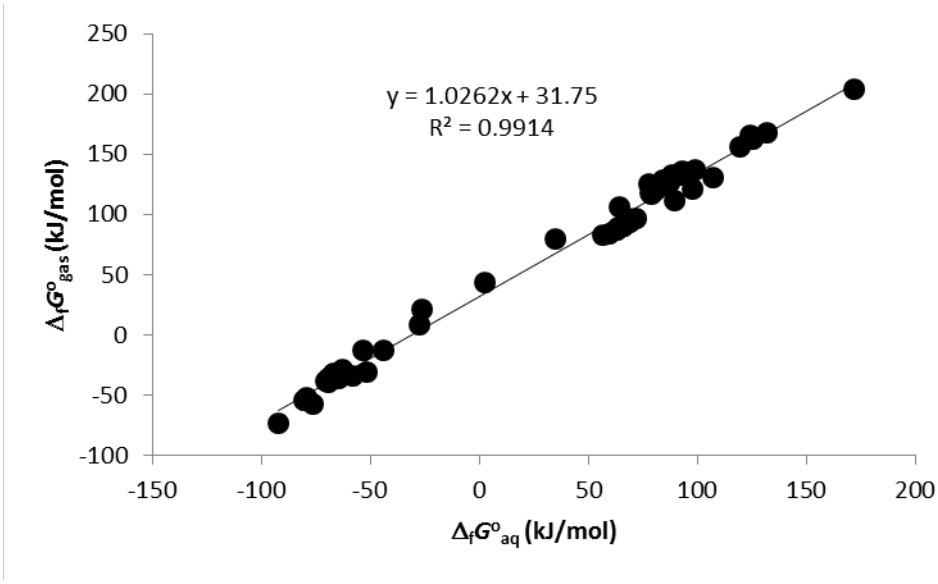
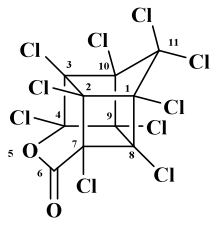


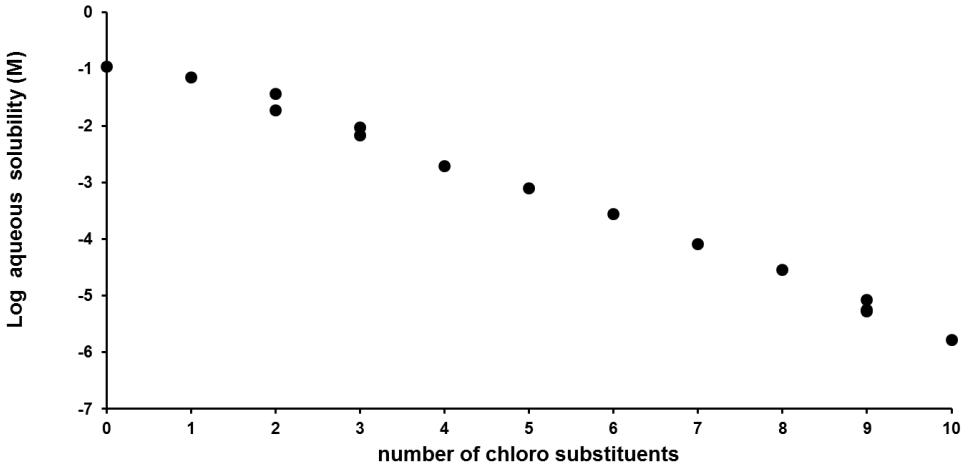
Figure SI-3. Structure of 'chlordecone lactone' plus its corresponding standard $\Delta_f G^o$ and $\Delta_f H^o$ values in kJ/mol (25 ^oC and 1 atm)



5-oxa-homochlordec-6-one
(chlordecone lactone)

compound	$\Delta_f G^o_{gas}$	$\Delta_f H^o_{gas}$	$\Delta_f G^o_{aq}$	$\Delta_f H^o_{aq}$
5-oxa-homochlordec-6-one	-222.1	-400.0	-239.6	-417.8

Figure SI-4. Estimated solubility of chlordecone congeners versus their degree of chlorination



* aqueous solubility calculated with EPA's SPARC online calculator (Arp, H. P. H. *et al*. Environ Sci Technol 2010, 44 (12), 4400-4401; Hilal, S. H. *et al.* QSAR Comb Sci 2004, 23 (9), 709-720; http://sparc.chem.uga.edu/sparc/).