Supporting Information

Arenium ions are not obligatory intermediates in electrophilic aromatic substitution

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Details of the Experiments

A number of experiments were conducted aimed at finding support for the principal conclusions from the theoretical studies on the mechanism and energetic of the anisole chlorination.

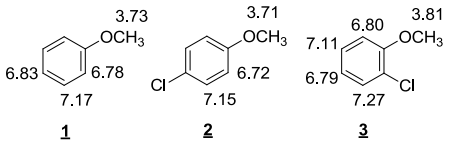
The course of the reaction was followed by recording spectra of the reaction mixture at various intervals. Two types of spectroscopic techniques were employed in analyzing the samples. FTIR spectra (Shimadzu FTIR 8400S) were recorded at 5 min intervals. The infrared technique proved, however, not sensitive enough and did not provide conclusive results with respect small amounts of side products besides the principal reaction products, which are *para*-chloroanisole and *ortho*-chloroanisole. Thus, NMR spectroscopy became the principal analytical technique in studying the chlorination process. ^{1}H (600.13 MHz) and ^{13}C (150.92 MHz) spectra were acquired on an AVANCE AV600 II+ NMR spectrometer. The spectra were recorded in CCl_4 at different temperatures with TMS as an internal standard for the ^{1}H and ^{13}C spectra. Unambiguous assignment of the signals was made on the basis of 1D and 2D gradient enhanced versions of COSY, TOCSY, NOESY, HSQC and HMBC experiments (Bruker pulse library programs: selno, selml, cosygpmfqf, dipsi2etgpsi, hsqcedetgpsisp2.2, and hmbcgplpndqf were applied). The programs of ACD/Labs (1), release 12, for predicting chemical shifts and the online tool of R. Stenutz (2) for the generalized $^{3}J_{HH}$ Karplus equation (3) for the J-couplings were employed.

Chlorination of anisole with chlorine at 25 °C. Anisole was dissolved in carbon tetrachloride at 25 °C in order to prepare solution with 1 mol/l concentration, while chlorine gas was introduced for 30 min.

Chlorination of anisole with chlorine at 5 °C. Chlorine gas was dissolved in carbon tetrachloride at 5 °C. Anisole was added in order to prepare a solution with 1 mol/l concentration (5 °C).

Chlorination of anisole with chlorine at −10 °C. Cl_2 and anisole were mixed in CCl_4 solvent at low temperature (−30 °C), the reaction is then followed by proton NMR spectroscopy. A series of NMR spectra were acquired at −10 °C. The reaction was followed for a period of 5 hours.

The identification and assignment of the *ortho* (**2**) and *para* (**3**) substitution products were trivial, despite their moderate (up to 0.15 ppm) chemical shift dependence on concentration The proton chemical shifts, measured in mixture 4, are depicted in Scheme S1.



Scheme S1. Proton chemical shifts for the principal products of anisole chlorination of in CCl_4 at 25 °C (reaction mixture 4, see Table 2 in the main text).

The stereochemistry of addition products **4** and **5** was unambiguously determined through detailed inspection of molecular models and comparison of predicted and experimental vicinal coupling constants and the corresponding to these constants dihedral angles. The experimental vicinal spin-spin coupling constants (H2-H3, 3.3Hz), (H3-H4, 9.0 Hz) and (H5-H6, 4.0 Hz) in **4** and (H2-H3, 5.1Hz), (H4-H5, 2Hz) and (H5-H6, 8.9Hz) in **5**, extracted from the proton NMR spectra correspond to dihedral angles 51, 159 and 39 for **4**,and 38, 63 and 158 for **5**. These values correlate quite well with the dihedral angles in the structures, depicted in Fig. S4, 68, 160 and 51 for **4** and 39, 66 and 159 - for **5**, respectively.

Brief explanation to the structure elucidation of compounds 4 and 5:

The experimental ^{1}H and ^{13}C NMR chemical shifts and coupling constants for compounds **4** and **5** are given in Table S1. They correspond well to the values, predicted by the ACD/Labs (1) program.

Unambiguous assignments of the signals were based on 1D and/or 2D gradient-enhanced versions of COSY, TOCSY, NOESY, HSQC, and HMBC experiments. The following observed signal connectivity's support unambiguous constitution of **4** and **5**, respectively:

2D DQFCOSY: Direct proton coupling partners were identified as follows: 4.41 (H-6, **5**):4.63 (H-5, **5**); 4.44 (H-6, **4**):4.5 (H-4,5, **4**); 4.5 (H-4,5, **4**):4.76 (H-3, **4**); 4.63 (H-5, **5**): 5.81 (H-3, **5**); 4.63 (H-2, **5**):5.84 (H-3, **5**); 4.76 (H-3, **4**):4.81 (H-2, **4**); 4.79 (H-2, **5**):5.84 (H-3, **5**); 5.81 (H-4, **5**):5.84(H-3, **5**) in full compliance with the coupling constants, extracted from the ^{1}H NMR spectra.

1D and 2D TOCSY: Detected connected spin systems constitute 4.81 (H-2, **4**) ↔ 4.76 (H-3, **4**) ↔ 4.5 (H-4,5, **4**) ↔ 4.44 (H-6, **4**) for **4** and 4.79 (H-2, **5**)↔5.82 (H-3,4, **5**)↔4.63 (H-5, **5**) ↔ 4.41 (H-6, **5**) for **5**, determined from several selective experiments with variable mixing time from 20 to 150 ms, in line with 2D dipsi experiment with mixing time of 150 ms.

HSQC: Observed direct heteronuclear (proton:carbon) correlation for the methoxy group in **4** is 3.60:55.06. Further detected correlations in **4** involve 4.76(H-3):56.41(C-3), 4.81(H-2):98.72(C-2) and 4.41(H-6):59.96(C-6). Correlations, detected in **5** include 3.54:50.67 for the methoxy couple, 4.41(H-6):64.06(C-6), 4.63(H-5):60.07(C-5), 4.79(H-2):55.57(C-2), 5.81(H-4):129.76(C-4) and 5.84(H-3):124.62(C-3).

HMBC: Surely detected are the following long-range connectivity's, that are in line with the structures elucidated and the assignments made: 3.54(C**H**$_3$O, **5**):104.13(C-6, **5**); 3.60 (C**H**$_3$O, **4**):151.29(C-1, **4**); 4.41 (H-6, **5**):60.07(C-5, **5**); 4.63(H-5, **5**):64.04(C-6, **5**); 4.63(H-5, **5**):124.62(C-3, **5**); 4.63(H-5, **5**):129.76(C-4, **5**); 4.79(H-2, **5**):104.13(C-6, **5**); 4.79(H-2, **5**):124.62(C-3, **5**); 4.79(H-2, **5**):129.76(C-4, **5**); 4.81(H-2, **4**):56.41(C-3, **4**); 5.81(H-4, **5**):64.06(C-6, **5**); 5.81(H-4, **5**):55.57(C-2, **5**); 5.84(H-4, **5**):60.07(C-5, **5**); 5.84(H-3, **5**):104.13(C-1, **5**).

The experimental proton and carbon chemical shifts correspond well to those calculated with the ACD chemical shift prediction program, based on empirically-determined additive increments (Table S1).

The relative configurations of the individual carbon atoms in **4** and **5** are determined using the available vicinal proton spin-spin coupling constants and the observed NOE enhancements. The experimental data allow unambiguous configuration assessment only for **5**. Representative calculation of the dihedral angles and energy in isomers with different relative configurations (Fig. S17) of the aliphatic carbon atoms in **5** is presented in Table S2. Only two isomers, which differ in the relative configuration of C-1 and have analogous structure of the remaining chain, agree with the spin coupling data. The C-1 configuration in the addition product **5** is assigned from the NOE data to have an equatorial methoxy group and an axial chlorine atom. The alternative configuration with an axial methoxy substituent should give rise to NOE not only to the H-2 and H-6 neighboring atoms, but also a relatively strong enhancement of H-5, that is not observed.

1D NOESY: Selective excitation of the methoxyl signal at 3.60 ppm leads to the following NOE features in **4**: 2.24% enhancement of the signal at 4.81 (H-2, **4**); 0.11% - at 4.76 (H-3, **4**) and 0.06% at 4.44 (H-6, **4**) ppm. Selective excitation of the methoxyl signal at 3.54 in **5** leads to 0.73% enhancements at 4.79 (H-2, **5**) and 0.05% at 4.41 (H-6, **5**) ppm.

Determination of the relative configuration of all carbon atoms in **4** is not possible from the available experimental data due to lack of the vicinal H-4-H-5 coupling constant value. $^{3}J_{45}$ could not be extracted from the spectra because the close chemical shift values of H-4 and H-5 give rise to a second order spin system, located in a spectral region with severe overlapping. The small value (4.0 Hz) of $^{3}J_{45}$ testifies for non-antiplanar comformation of protons 4 and 5. Thus, three possible diastereomers could not be distinguished on the basis of the experimental data. The axial H-3 and the antiperiplanar disposition of the vicinal H-4 are unambiguously deduced from the values of the coupling constants $^{3}J_{23}$ and $^{3}J_{34}$. Thus, a tentative assignment of the

stereochemistry of **4** also is based on their computed energies. The structure of **4** shown in Fig. S4 has the lowest B2PLYP+D3/6-311+G(2d,2p) energy of the three possible diastereomers. The structures of these isomers and their computed energies are shown in Fig. S16 and Table S3.

Further NMR experiments were conducted at 5 °C and at −10 °C following the same procedure. The latter were more revealing. CCl_4 solutions of Cl_2 and of anisole were mixed at −30 °C and the reaction was followed for 5 hours at −10 °C. Representative NMR spectra of the reaction mixture taken at 5', 15', 1h, 2h, 3h, 4h, and 5h after the start of the reaction, when no appreciable remaining quantity of anisole could be detected are compared in Figs. S13 and S14. After one hour reaction time, appreciable amounts of compounds **2**, **3**, **4** and **5**, are detected as main components at room temperature, their quantity further increases with time. A number of additional products also are detected in smaller amounts, some of them forming and disappearing during the reaction. No unambiguous proof for the presence of an addition product of one molecular chlorine to anisole could be obtained, but cannot be excluded. A small doublet signal around 5.2 ppm (J = 6.9Hz) was detected in the reaction mixture 10 minutes after the start of the reaction (at −10 °C), its maximum quantity was 30 minutes, but it fully disappeared in 4 hours. The signal at 5.2 ppm could correspond to the olefinic proton *ortho* to the methoxy group in structure **6** (Fig. S15). All other protons in this structure have lower intensities because of the splitting and could not be detected unambiguously due to overlap with other signals.

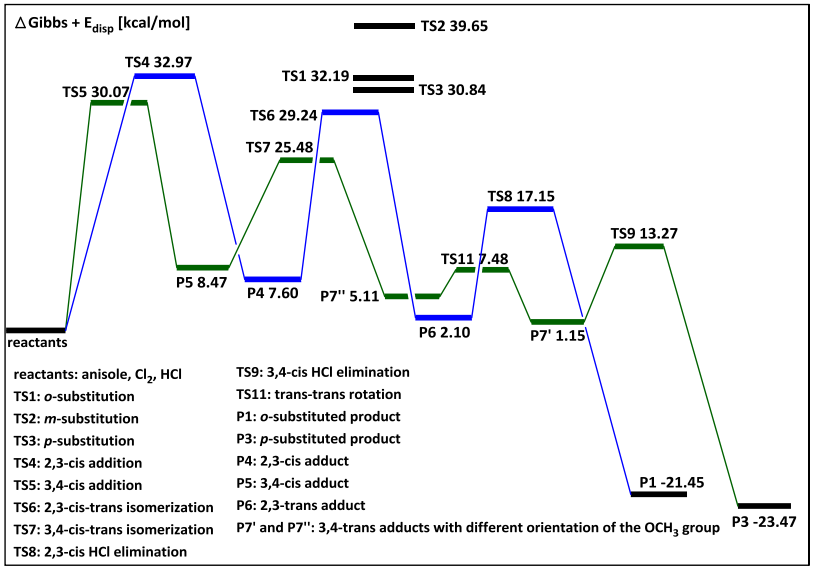


Fig. S1. Computed potential energy surface (PES) for anisole-Cl_2, catalyzed by HCl, reactions in isolation (gas-phase) at B3LYP/6-311+G(2d,2p).

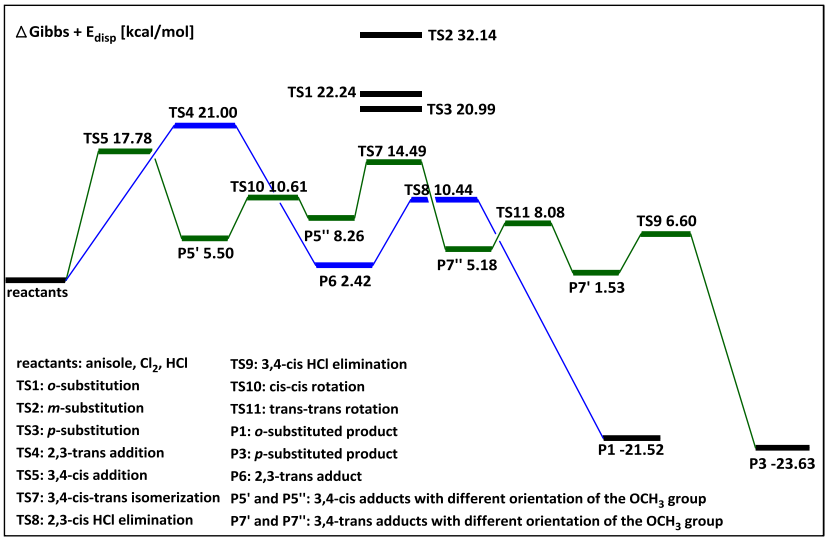
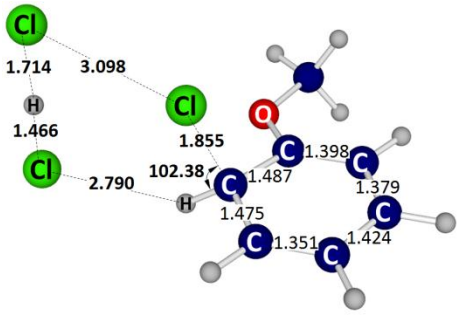
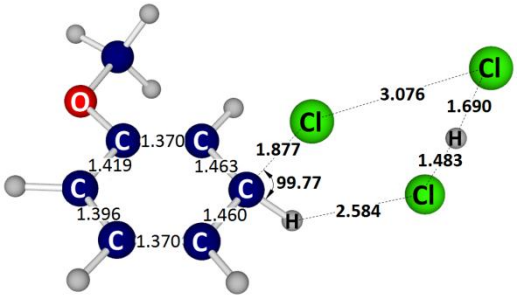


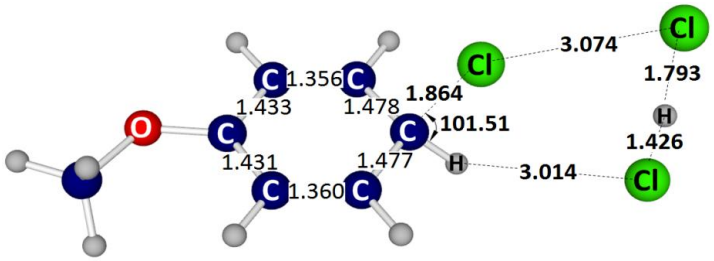
Fig. S2. Computed potential energy surface (PES) for catalyzed by HCl anisole-Cl_2 reactions in simulated CCl_4 solvent at B3LYP/6-311+G(2d,2p).



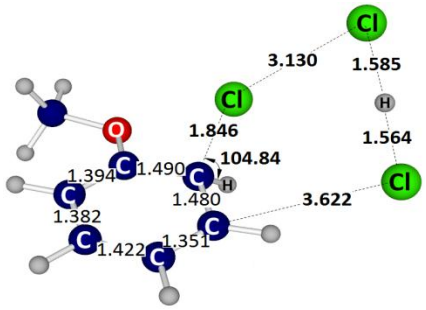
***o*-substitution TS1** (99.3 *i*)



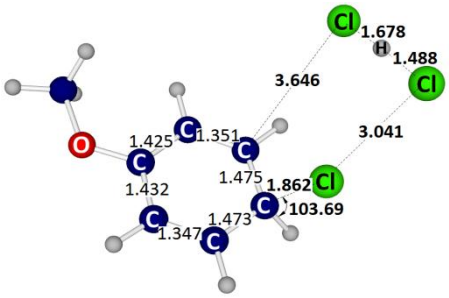
***m*-substitution TS2** (215.8 *i*)



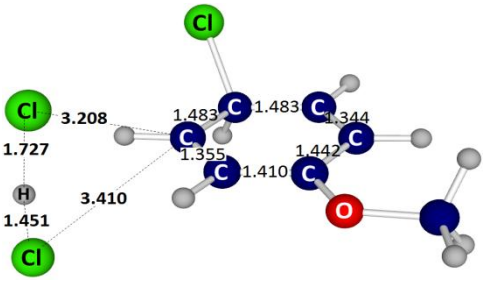
***p*-substitution TS3** (59.2 *i*)



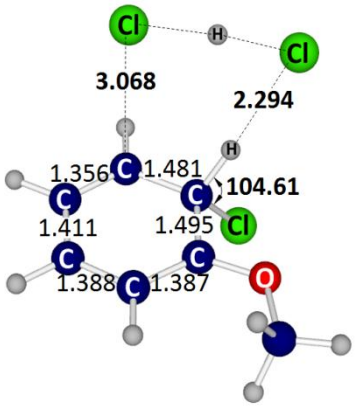
2,3-trans addition TS4 (299.4 *i*)



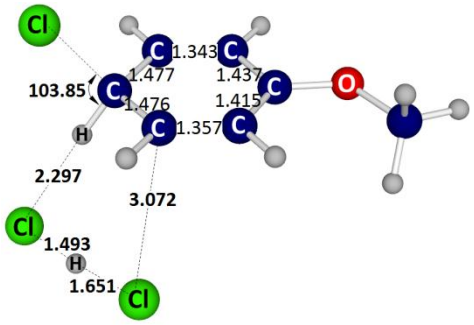
3,4-cis addition TS5 (119.3 *i*)



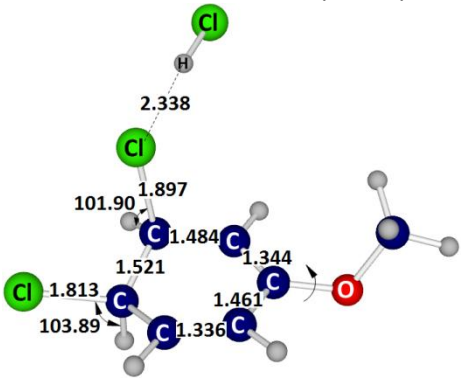
3,4-cis-trans isomerization TS7 (52.6 *i*)



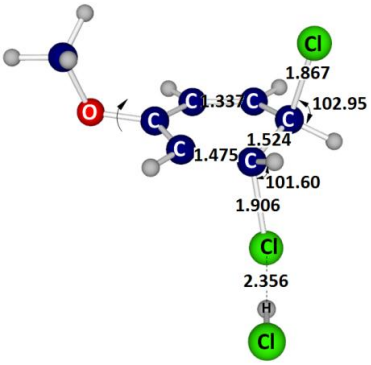
2,3-cis elimination TS8 (147.4 *i*)



3,4-cis elimination TS9 (82.9 *i*)



cis-cis rotation TS10 (70.1 *i*)



trans-trans rotation TS11 (95.1 *i*)

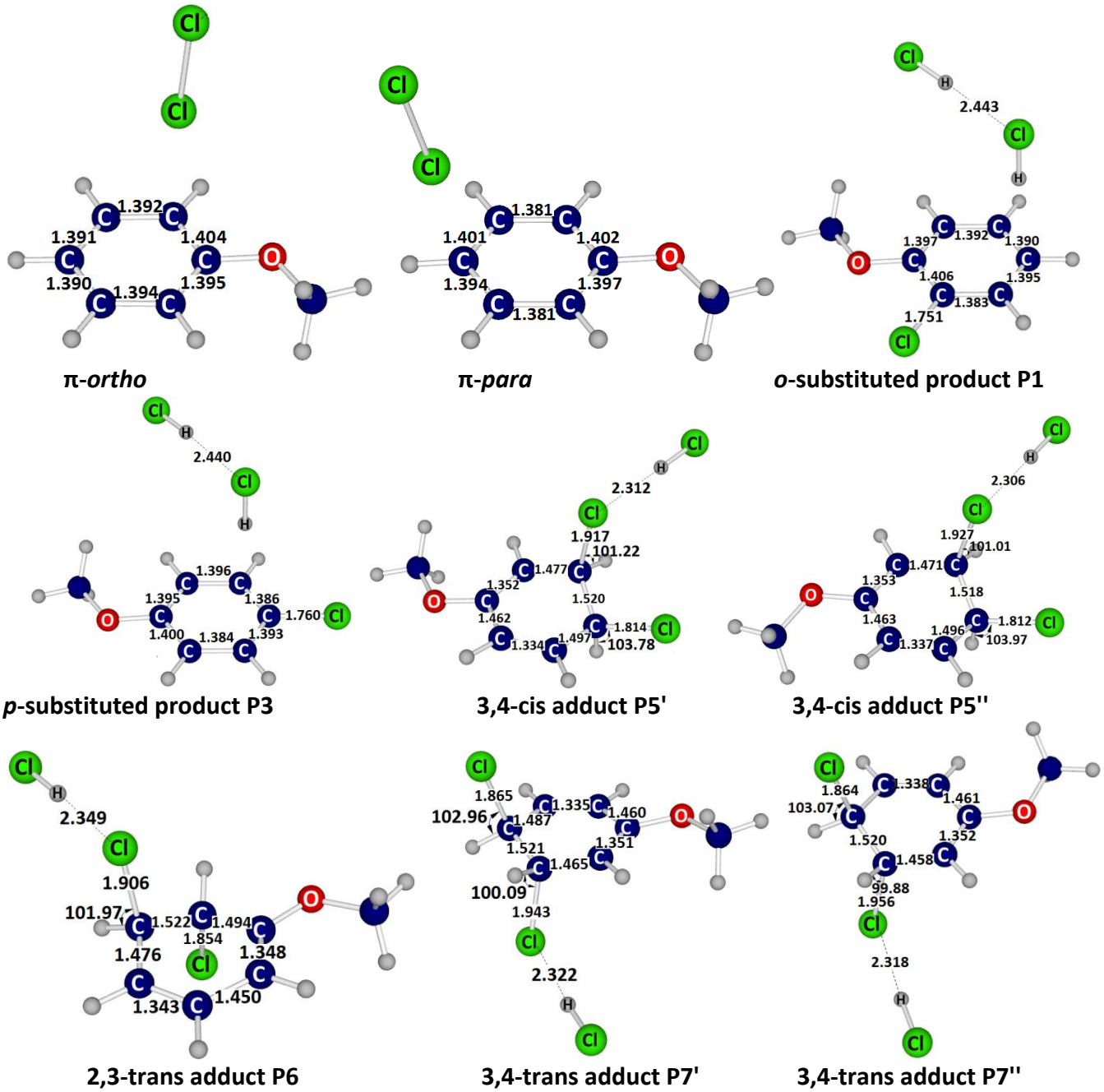
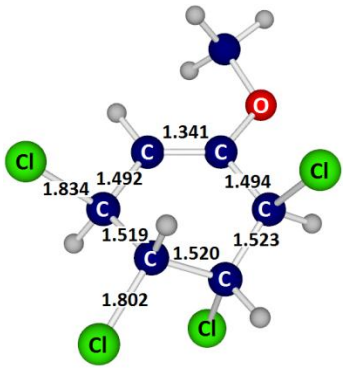
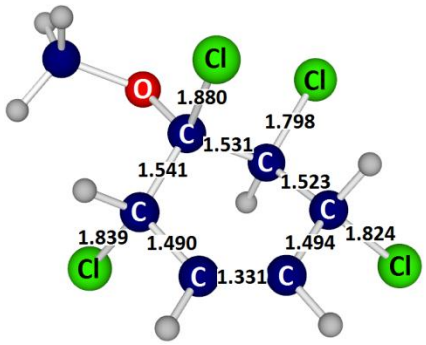


Fig. S3. Geometries of the transition states, π-complexes, **P1**, **P3**, **P5**, **P6** and **P7** for HCl-catalyzed anisole-Cl_2 reactions, in simulated CCl_4 solution at B3LYP/6-311+G(2d,2p) (bond lengths in Å, bond angles in degrees). **TS3** was optimized at B3LYP/6-31+G(d,p). **TS7** was optimized in isolation (gas-phase) at B3LYP/6-311+G(2d,2p). Cis-trans isomerization, elimination transition states, and adducts leading to *m*-substituted product formation are not included.

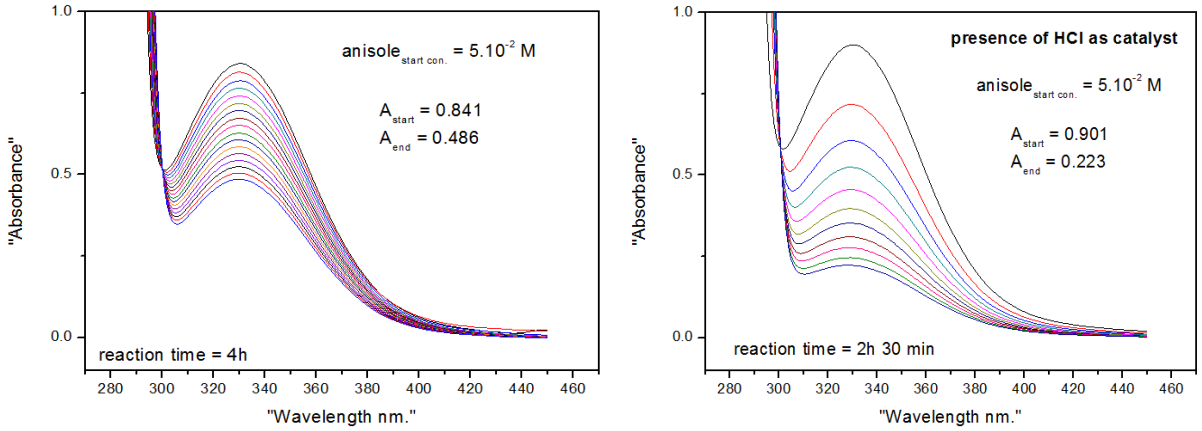


4



5

Fig. S4. Structures of **4** and **5** by-products formed during the chlorination of anisole in CCl_4. Geometries of the anisole-Cl_2 addition products for were optimized in simulated CCl_4 solution at B2-PLYP/6-311+G(2d,2p).



A B

Fig. S5. Gradual consumption of Cl_2 (via its band at 330 nm) during the reaction with anisole (at 25 °C) in absence of added HCl (A, initial Cl_2 concentration: 8.10^{-3} mol/l, anisole 5.10^{-2} mol/l) and when HCl is added to the reaction mixture prior to Cl_2 flow (B, initial Cl_2 concentration: 6.10^{-3} mol/l, anisole 5.10^{-2} mol/l). The spectra registration intervals were 15 minutes for both A and B.

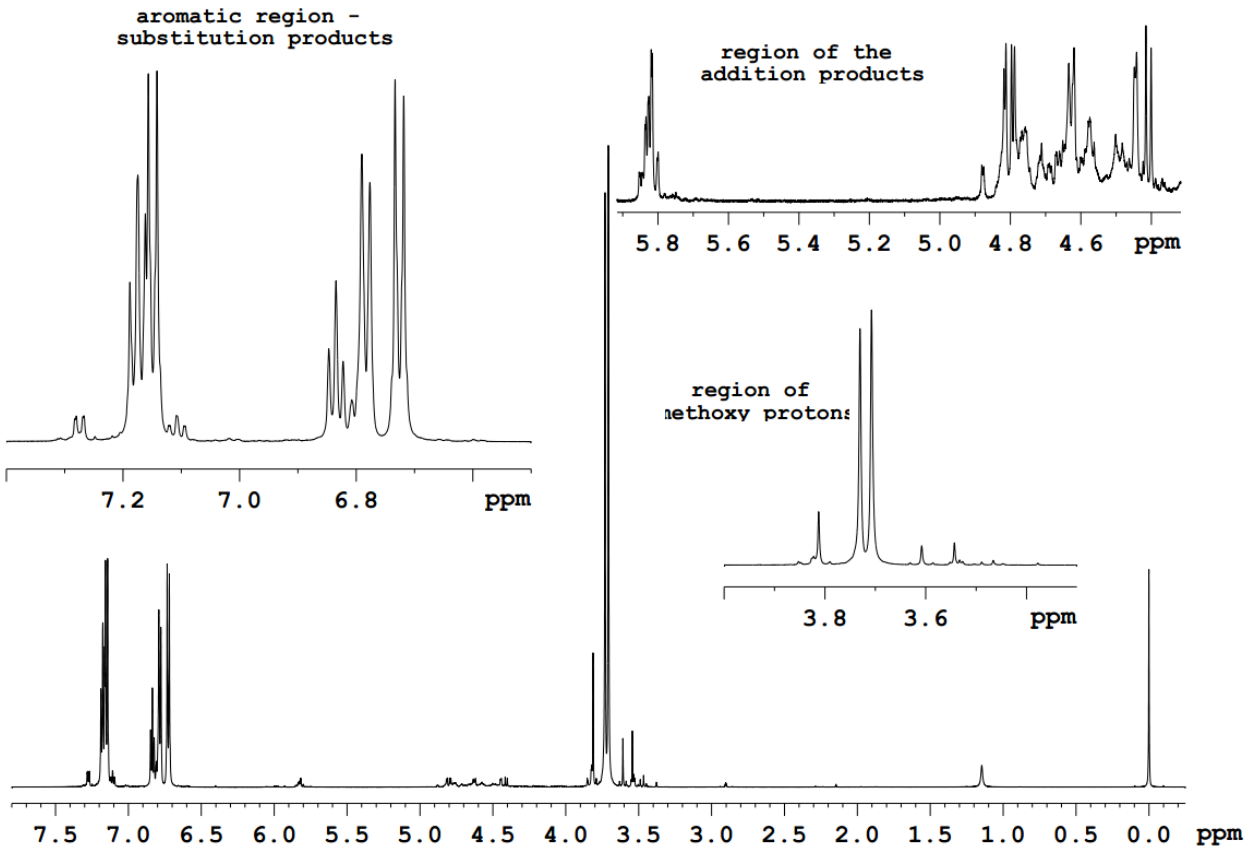


Fig. S6. ^{1}H NMR spectrum of mixture 4 from 0 to 7.5 ppm. The positions of the aromatic protons cover a range from 6.6 to 7.4 ppm. The signals for the protons of the addition products were found in the range 4.4 – 5.9 ppm. The signal of the methoxy group appears at 3.4 – 4 ppm. The spectra were recorded at 5 °C.

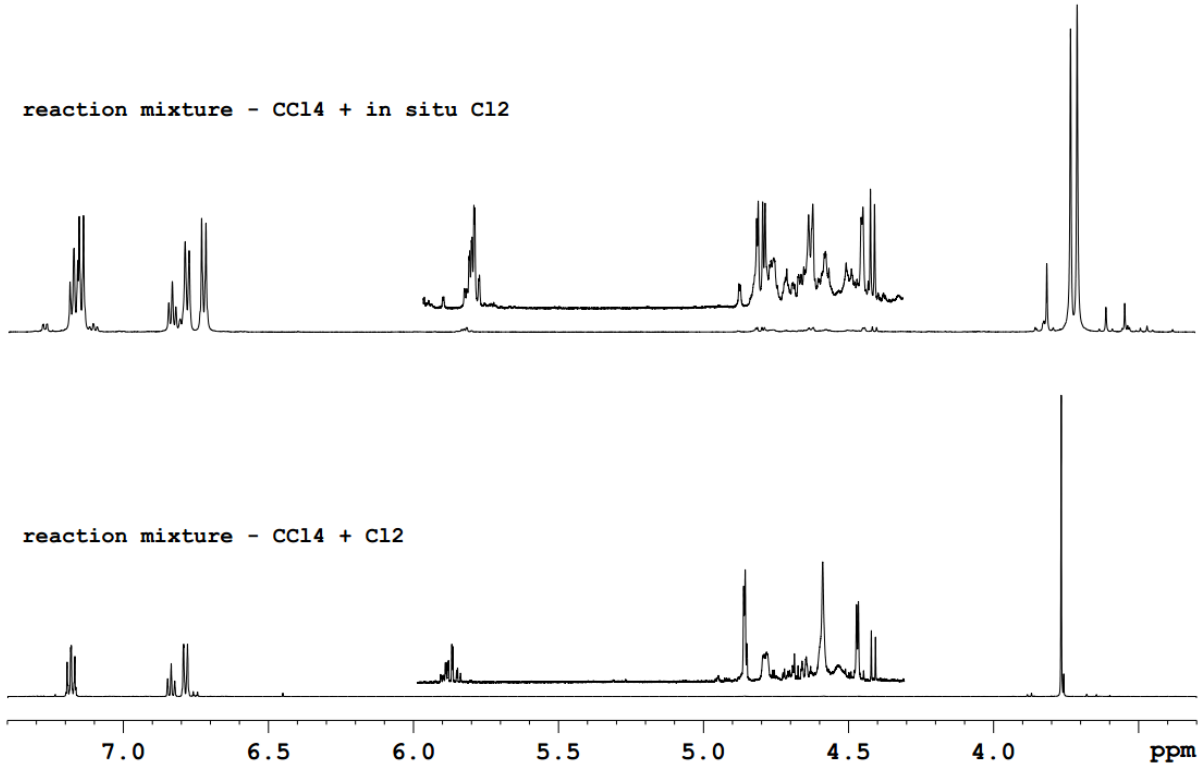


Fig. S7. ^{1}H NMR spectra of mixtures 1 and 4. For mixture 1 the ^{1}H NMR spectrum was recorded at 25 °C. For mixture 4 the ^{1}H NMR spectrum was recorded at 5 °C.

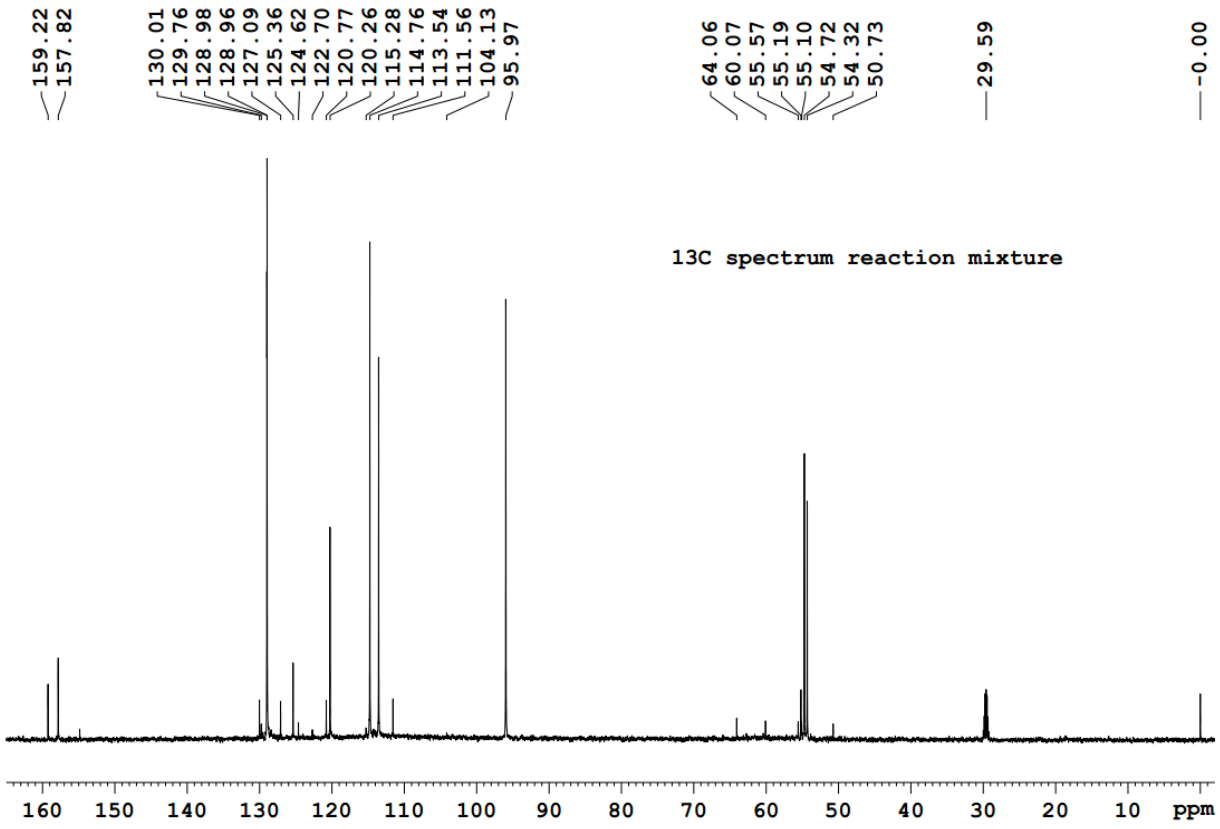


Fig. S8. ^{13}C NMR spectrum of mixture 4. The spectrum was recorded at 5 °C.

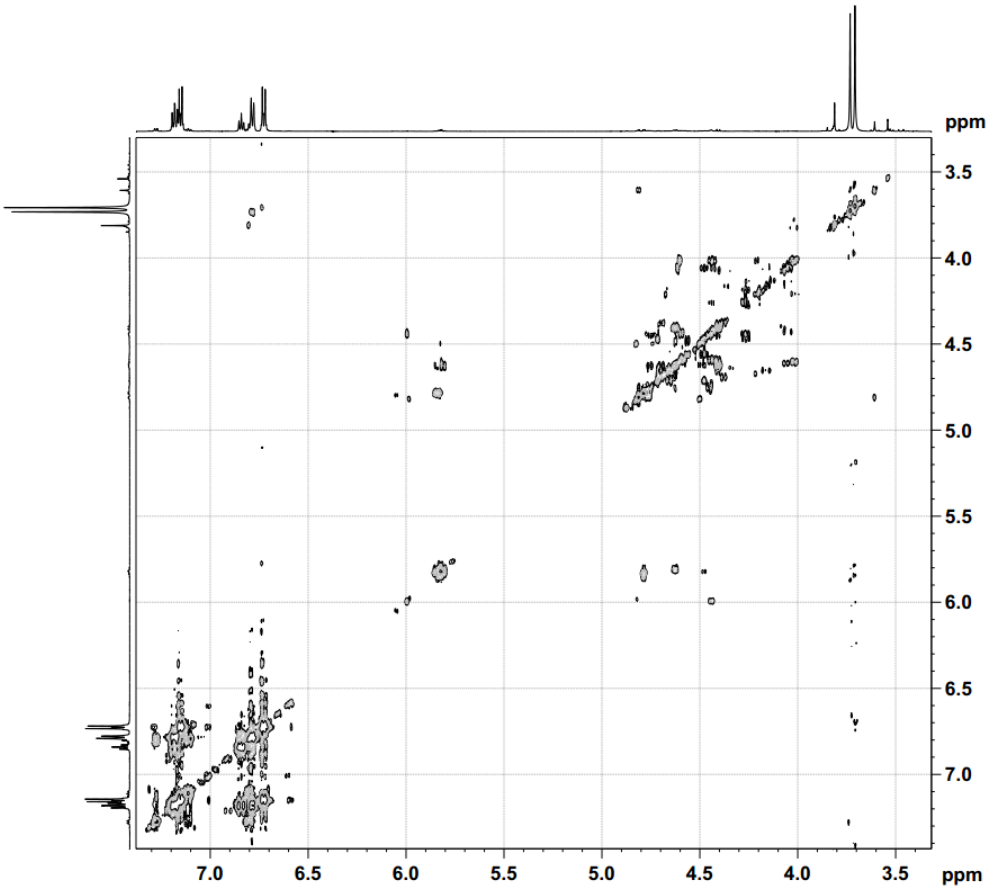


Fig. S9. Double quantum filtered ^{1}H-^{1}H COSY of mixture 4. The spectrum was recorded at 5 °C.

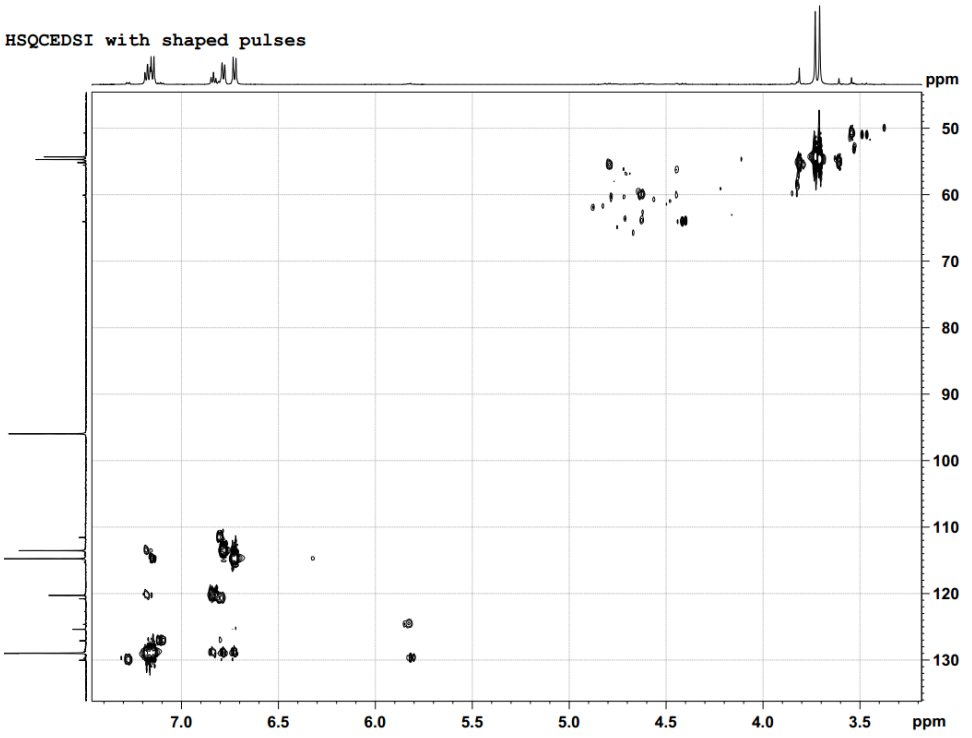


Fig. S10. 2D-Heteronuclear ^{1}H-^{13}C HSQC of mixture 4. The spectrum was recorded at 5 °C.

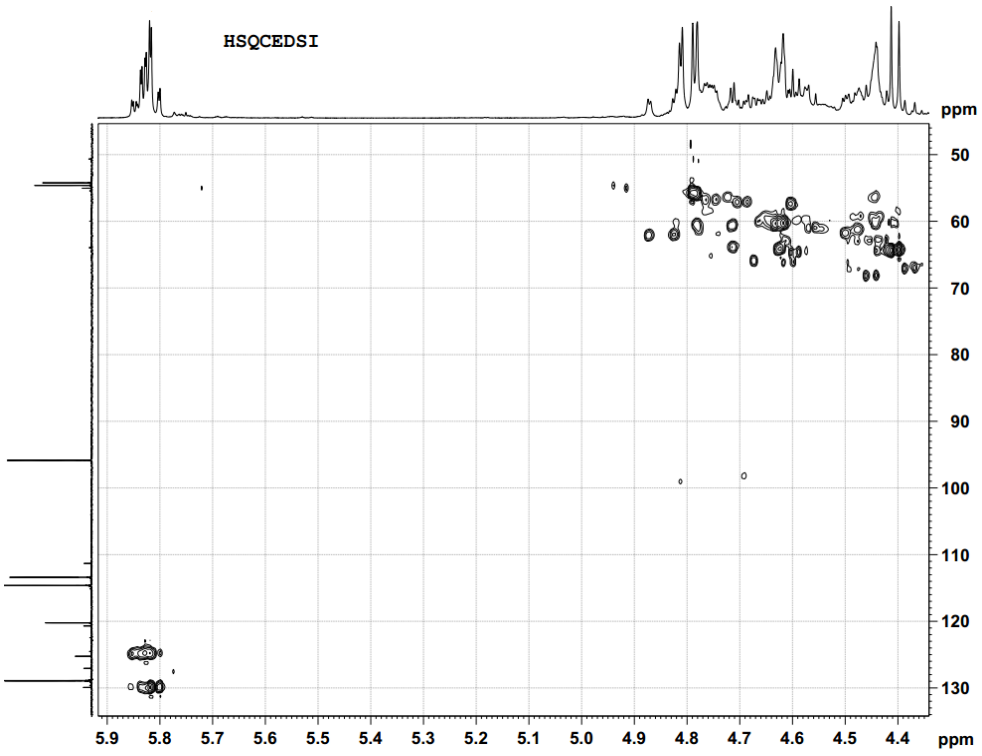


Fig. S11. 2D-Heteronuclear ^{1}H-^{13}C HSQC of mixture 3 – expansion of the region for the addition products. The spectrum was recorded at 25 °C.

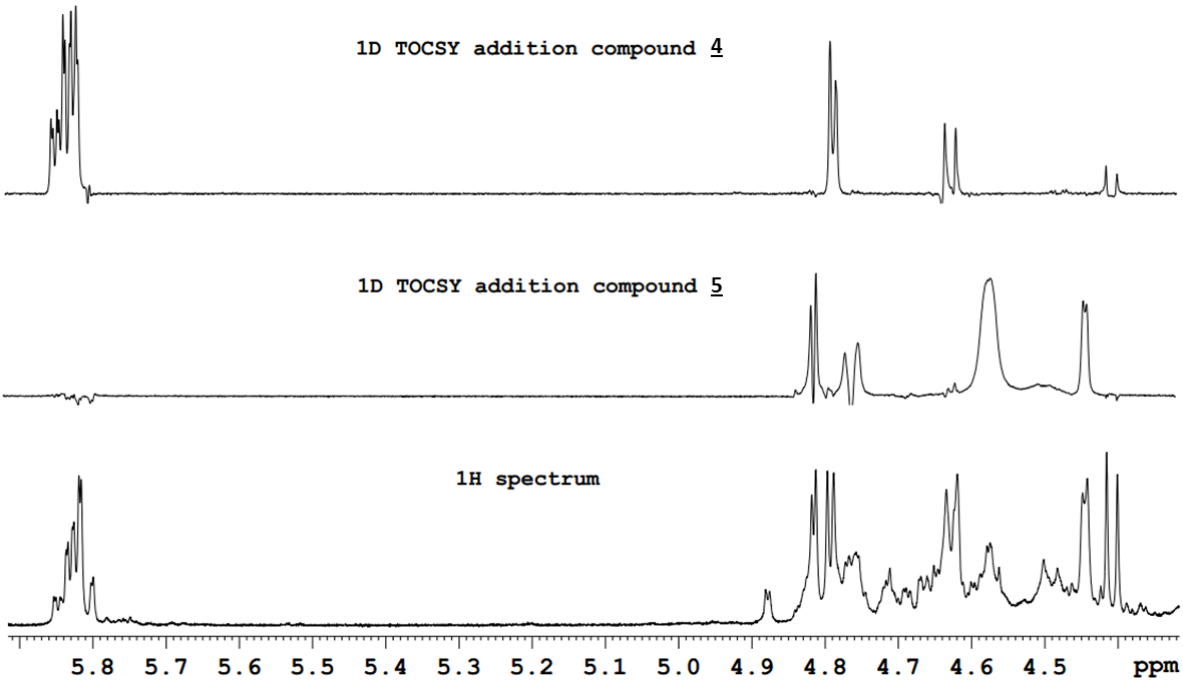


Fig. S12. Region from 4 to 6 ppm of a) 1D TOCSY spectrum for addition product **4** and b) **5** and c) ^{1}H NMR spectrum.

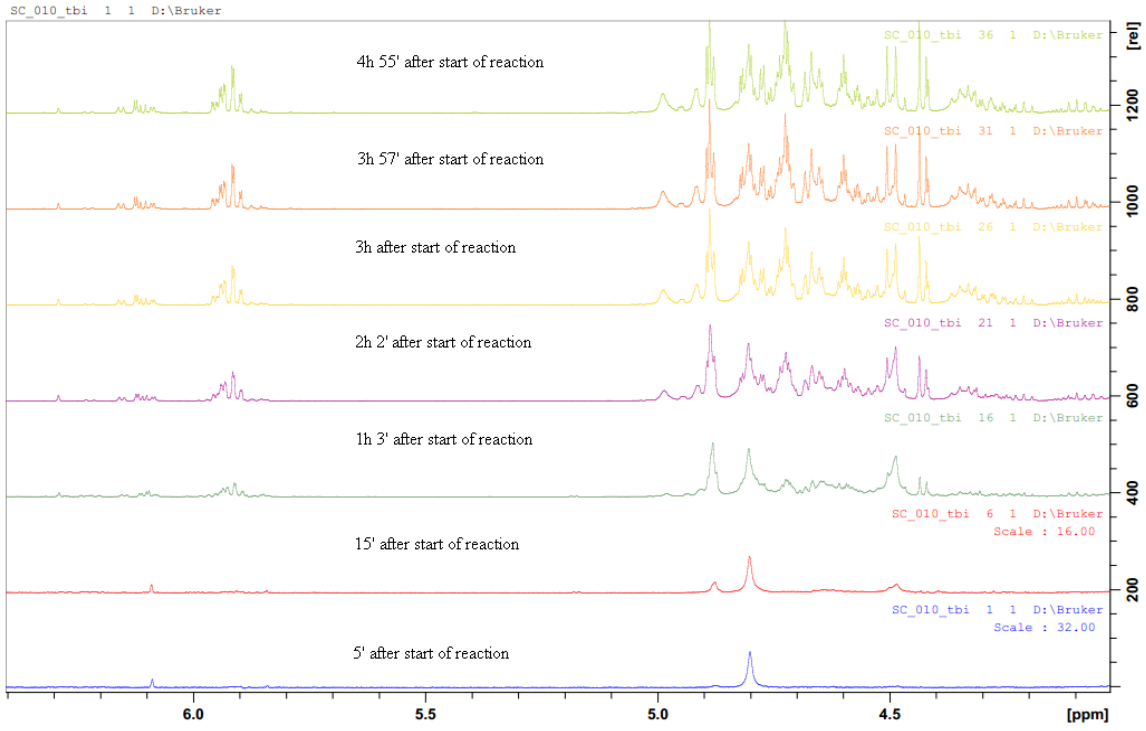


Fig. S13. ^{1}H NMR spectra of anisole chlorination at −10 °C in the 4 – 6 ppm range. The initial concentration of anisole was 1.5 mol/l.

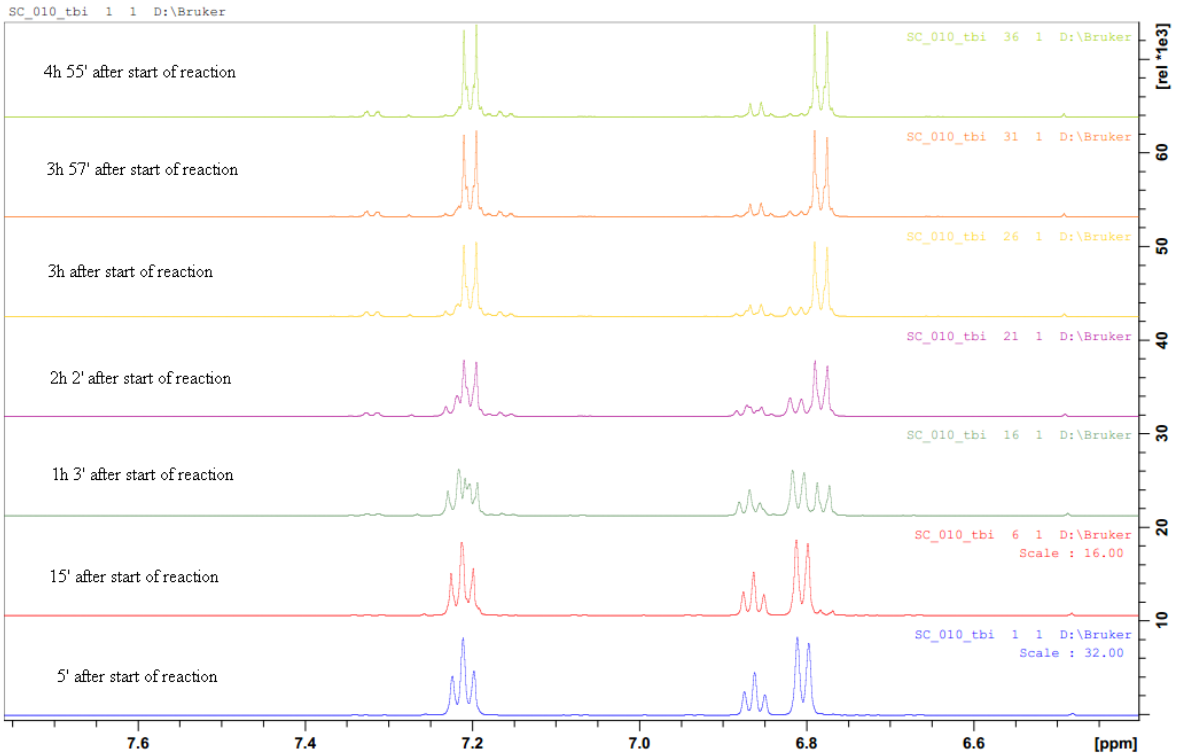


Fig. S14. ^{1}H NMR spectra of aromatic region of experiment conducted in −10 °C in the range 6.4 – 7.6 ppm. The initial concentration of anisole is 1.5 mol/l.

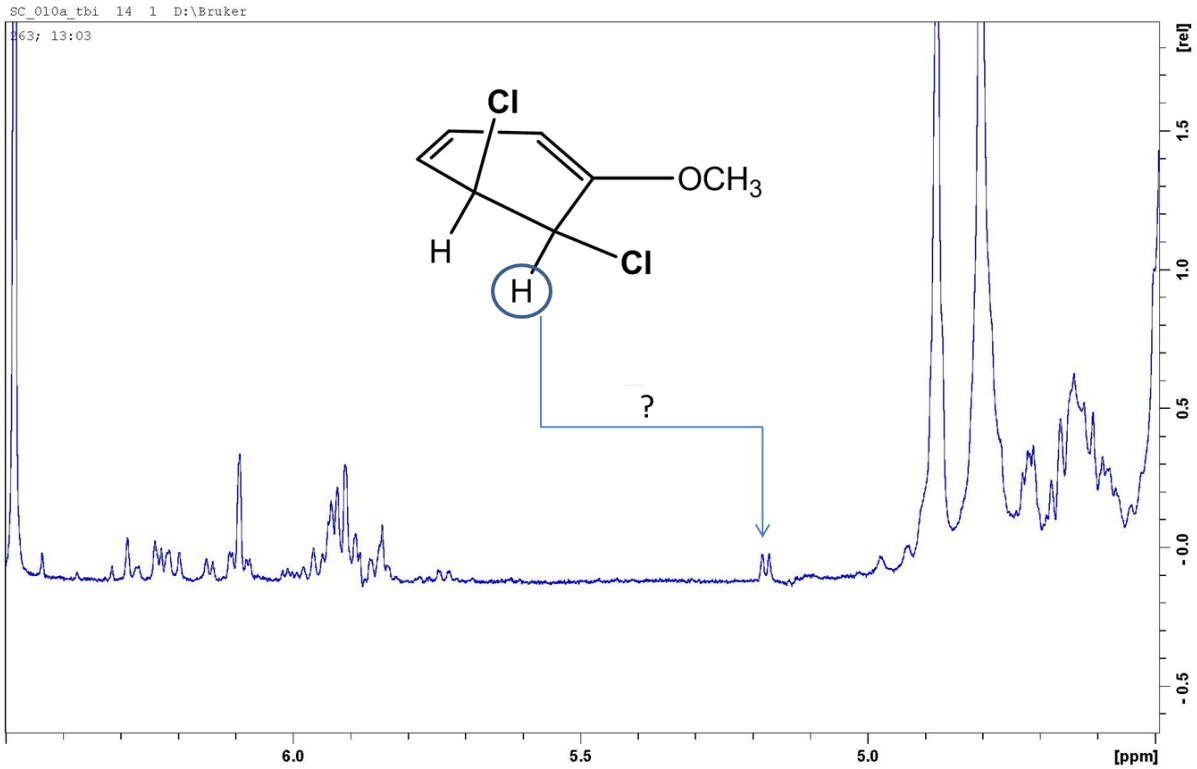
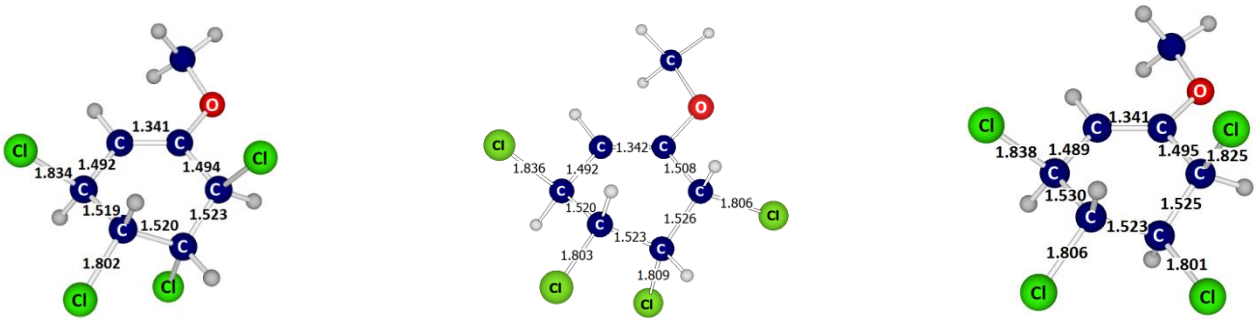


Fig. S15. Experimental ^{1}H NMR spectrum in the range 4.5 – 6.5 ppm with maximum quantity of the doublet at 5.18 ppm. The spectrum was recorded at −10 °C.



4 **4 (2)** **4 (3)**

Fig. S16. Structures of **4**, **4 (2)** and **4 (3)** in simulated CCl_4 solution at B2-PLYP/6-311+G(2d,2p).

Table S1. ^{1}H and ^{13}C NMR chemical shifts and coupling data for compounds **4** and **5**.

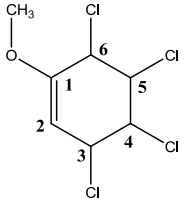
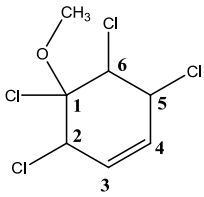
		^{1}H and ^{13}C NMR chemical shifts and coupling data from experiment	ACD chemical shift prediction
(**4**)		151.29 – C1 3.60s, 55.06 – CH_3O 4.81 d (3.3), 98.72 – C2 4.76 dd (9.3; 3.3), 56.41 – C3 4.5–4.6 m, 2H, 59.54 and 60.58, C4+C5 4.44 d (4.0), 59.96 – C6	152.44 – C1 3.73, 56.12 – CH_3O 5.31, 101.45 – C2 4.85, 56.17 – C3 4.08, 4.19, 2H, 62.85 and 62.52, C4+C5 4.42, 58.60 – C6
(**5**)		104.13 – C1 3.54 s, 50.67 – CH_3O 4.79 d (5.1), 55.57 – C2 5.84 ddd (10.0; 5.1; 1.8), 124.62 – C3 5.81 dd (10.0; 2.0), 129.76 – C4 4.63 (8.9; 1.9), 60.07– C5 4.41 d(8.9), 64.06 – C6	104.75 – C1 3.36, 54.55 – CH_3O 4.72, 58.95 – C2 5.94, 125.25 – C3 6.12, 125.02 – C4 4.80, 55.60 – C5 4.37, 64.79 – C6

Table S2. Dihedral angles (φ), MMFF94 energies given by SPARTAN'08 (E, kcal/mol) of representative conformers for several diastereoisomers with different relative configurations, compared with the experimental and theoretically determined data for compound **5**.

φ[a,b]	from exp.[c]	**5** R1*S2*R5*S6*				**5** S1*S2*R5*S6*		**5** S1*R2*R5*S6*			**5** S1*S2*S5*S6*			**5** S1*R2*S5*R6*		**5** S1*R2*S5*R6*	
		Theor.[d]	M1[f]	M2	M3	M1	M2	M1	M2	M3	M1	M2	M3	M1	M2	M1	M2
2-3	38	39	38	35	36	38	40	**78**[b]	**83**	**76**	**77**	**82**	**75**	43	45	**76**	**82**
4-5	63	68	66	64	64	67	68	68	65	64	48	50	53	456	46	47	50
5-6	158	159	156	153	154	158	162	165	165	155	**47**	**44**	**36**	**79**	**77**	**75**	**79**
E			68.1	70.6	72.1	68.9	70.3	71.7	72.0	75.8	75.1	76.9	81.8	73.1	73.2	71.6	73.8
%[e]			98.4	1.5	0.1	91.3	8.7	62.3	37.7	0.1	95.3	4.7	0	54.2	45.8	97.6	2.4

[a] Dihedral angle between vicinal protons, as numbered in Table S1; [b] Dihedral angles in red differ by more than 35 gedrees from experiment in conformers; [c] Dihedral angles, calculated from the corresponding observed in this work vicinal coupling constants according to Haasnoot et al. (68); [d] From B2PLYP/6-311+G(2d,2p) computations; [e] Conformer population based on relative E's; [f] Mi stands for the lowest energy conformers of each diastereomer, calculated by the conformer distribution routine.

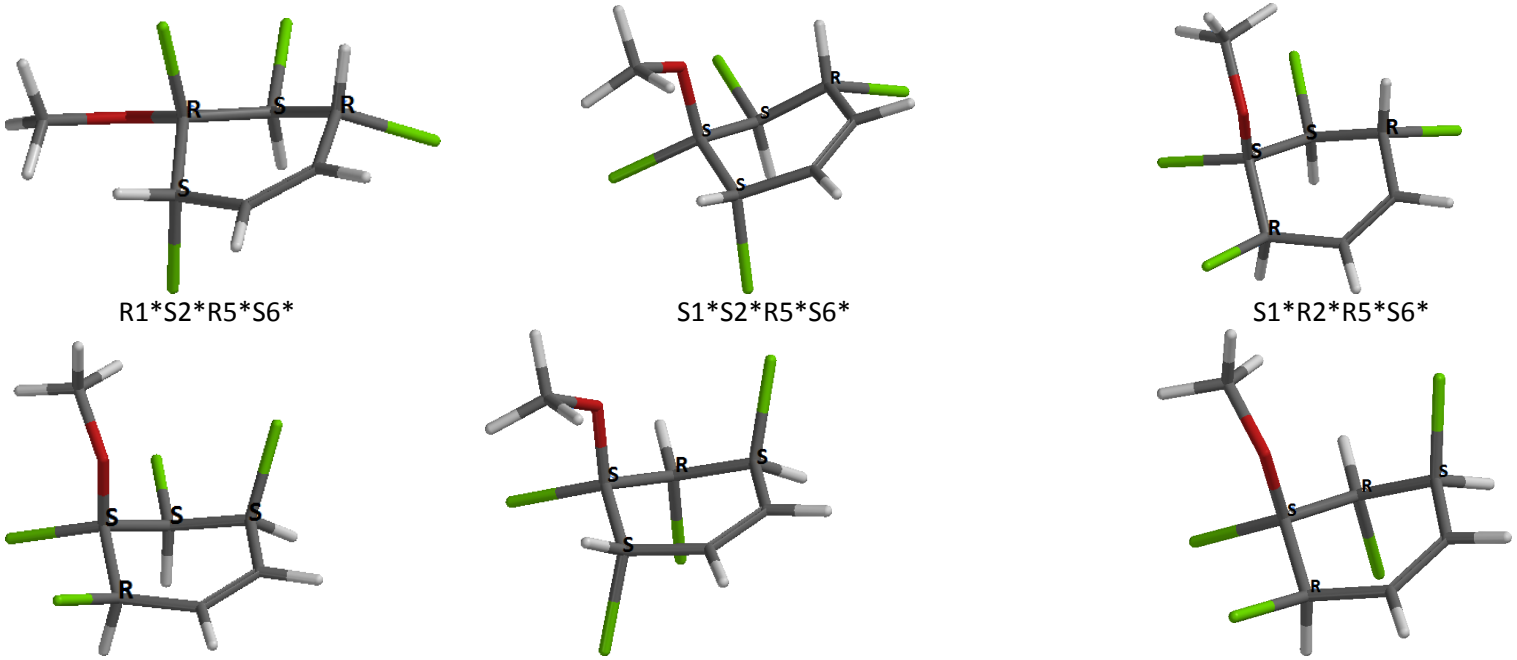


Fig. S17. Structure of a representative set of diastereoisomers of **5** with different relative configuration.

Table S3. Dihedral angles (φ, in degrees) and energies (B2PLYP/6-311+G(2d,2p)) of **4** and its configurational isomers **4(2)** and **4(3)**.

φ	exp.[a]	**4**[b]	**4(2)**	**4(3)**
2-3	51	66	68	61
3-4	159	159	160	151
5-6	39	69	51	55
E [hartree]		-2186.84525	-2186.83856	-2186.84144

a) Calculated from the corresponding observed ^3J (68)

b) Structure **4** is represented in Fig. S4.

Table S4. Electronic (E_{el}), thermal correction to Gibbs Free Energy, ZPE, and E_{disp} Energies as well as NImag of species involved in the catalyzed by HCl anisole-Cl_2 reaction in the gas phase, computed at RB3LYP/6-311+G(2d,2p) with stable wavefunction, no diradical character.

Species	Description	E_{el} [a.u.]	Thermal corr. [a.u.]	ZPE [kcal/mol]	E_{disp} [kcal/mol]	NImag [freq cm^{-1}]
anisole		-346.88122	63.81	83.31	-5.92	0
Cl_2		-920.41859	-12.94	0.77	-0.02	0
HCl		-460.83630	-7.05	4.17	-0.002	0
π-*ortho*		-1267.30325	58.73	84.44	-9.00	0
π-*para*		-1267.30366	58.87	84.49	-8.75	0
TS1	*o*-substitution	-1728.10300	61.30	87.95	-11.99	1 (*i*=579.0)
TS2	*m*-substitution	-1728.08929	59.93	87.39	-11.77	1 (*i*=846.5)
TS3	*p*-substitution	-1728.10588	61.34	88.17	-11.58	1 (*i*=365.3)
TS4	2,3-cis addition	-1728.10186	61.89	88.23	-12.53	1 (*i*=517.0)
$TS4_{meta}$[a]	2,3-cis addition	-1728.09124	61.81	88.13	-12.88	1 (*i*=366.7)
TS5	3,4-cis addition	-1728.10649	61.65	88.19	-12.28	1 (*i*=580.2)
$TS5_{meta}$[a]	3,4-cis addition	-1728.08920	61.42	87.70	-12.35	1 (*i*=826.7)
TS6	2,3-cis-trans	-1728.10686	61.86	88.69	-13.09	1 (*i*=59.8)
TS7	3,4-cis-trans	-1728.11307	61.95	88.82	-13.03	1 (*i*=52.6)
$TS7_{meta}$[a]	3,4-cis-trans	-1728.09613	61.09	87.68	-13.18	1 (*i*=223.9)
TS8	2,3-cis HCl eli	-1728.12564	62.20	88.12	-13.73	1 (*i*=275.2)
$TS8_{meta}$[a]	2,3-trans HCl eli	-1728.09620	62.65	89.05	-14.24	1 (*i*=40.8)
TS9	3,4-cis HCl eli	-1728.13245	62.29	88.24	-13.42	1 (*i*=206.5)
$TS9_{meta}$[a]	3,4-cis HCl eli	-1728.11570	61.98	87.50	-13.59	1 (*i*=354.2)
TS11	trans-trans rot.	-1728.14313	62.78	90.34	-13.01	1 (*i*=89.0)
P1	*o*-product	-1728.18290	57.87	87.65	-12.07	0
P2	*m*-product	-1728.18557	57.64	87.48	-12.06	0
P3	*p*-product	-1728.18516	57.28	87.51	-12.07	0
P4	2,3-cis adduct	-1728.14422	63.51	90.82	-12.93	0
P5''	3,4-cis adduct	-1728.14093	62.12	90.45	-12.74	0
$P5_{meta}$[b]	3,4-cis adduct	-1728.14477	62.38	90.50	-13.01	0
P6	2,3-trans adduct	-1728.15192	63.01	90.96	-13.10	0
P7'	3,4-trans adduct	-1728.15364	63.29	91.00	-13.25	0
P7''	3,4-trans adduct	-1728.14609	62.07	90.66	-12.80	0
$P7_{meta}$[b]	3,4-trans adduct	-1728.15235	62.98	90.91	-12.90	0

a) High energy transition states, associated with the formation of adducts, in which the orientation of the HCl leads to formation of *m*-substituted product;

b) High energy adducts, leading to *m*-substituted product formation.

Table S5. Electronic (E_{el}), thermal correction to Gibbs Free Energy, ZPE, and E_{disp} Energies as well as NImag of species involved in the catalyzed by HCl anisole-Cl_2 reaction in simulated CCl_4 solvent, computed at RB3LYP/6-311+G(2d,2p) with stable wavefunction, no diradical character.

Species	Description	E_{el} [a.u.]	Thermal corr. [a.u.]	ZPE [kcal/mol]	E_{disp} [kcal/mol]	NImag [freq cm^{-1}]
anisole		-346.88309	63.80	83.30	-5.92	0
Cl_2		-920.41908	-12.94	0.76	-0.02	0
HCl		-460.83758	-7.07	4.15	-0.002	0
π-*ortho*		-1267.30568	59.01	84.43	-9.07	0
π-*para*		-1267.30613	59.10	84.46	-8.82	0
TS1	*o*-substitution	-1728.12397	62.01	88.74	-11.81	1 (*i*=99.3)
TS2	*m*-substitution	-1728.10594	60.51	87.77	-11.72	1 (*i*=215.8)
TS3[a]	*p*-substitution	-1728.12778	62.57	89.43	-11.23	1 (*i*=59.2)
TS4	2,3-trans addition	-1728.12433	60.90	88.07	-11.71	1 (*i*=299.4)
$TS4_{meta}$[b]	2,3-trans addition	-1728.10749	60.28	87.42	-12.16	1 (*i*=422.4)
TS5	3,4-cis addition	-1728.13094	61.62	88.68	-11.50	1 (*i*=119.3)
$TS5_{meta}$[b]	3,4-cis addition	-1728.10564	60.15	87.38	-11.97	1 (*i*=612.6)
TS7[c]	3,4-cis-trans	-1728.13428				
$TS7_{meta}$[b]	3,4-cis-trans	-1728.11264	60.59	87.79	-12.78	1 (*i*=47.4)
TS8	2,3-cis HCl eli	-1728.13906	61.27	88.29	-13.40	1 (*i*=147.4)
$TS8_{meta}$[b]	2,3-cis HCl eli	-1728.12433	62.44	88.28	-14.13	1 (*i*=115.4)
TS9	3,4-cis HCl eli	-1728.14637	61.63	88.49	-13.01	1 (*i*=82.9)
$TS9_{meta}$[b]	3,4-cis HCl eli	-1728.12515	61.88	87.78	-13.35	1 (*i*=196.5)
TS10	cis-cis rot.	-1728.14181	62.61	90.08	-12.84	1 (*i*=70.1)
TS11	trans-trans rot.	-1728.14681	63.07	90.27	-12.70	1 (*i*=95.1)
P1	*o*-product	-1728.18593	56.98	87.54	-11.66	0
P2	*m*-product	-1728.18856	56.83	87.38	-11.14	0
P3	*p*-product	-1728.18783	56.00	87.36	-11.60	0
P5'	3,4-cis adduct	-1728.15184	63.51	90.68	-12.56	0
P5''	3,4-cis adduct	-1728.14558	62.35	90.39	-12.57	0
$P5_{meta}$[d]	3,4-cis adduct	-1728.14903	63.28	90.70	-12.52	0
P6	2,3-trans adduct	-1728.15556	63.07	90.84	-12.87	0
$P6_{meta}$[d]	2,3-trans adduct	-1728.14840	62.94	90.63	-13.54	0
P7'	3,4-trans adduct	-1728.15713	63.15	90.86	-12.85	0
P7''	3,4-trans adduct	-1728.15043	62.45	90.56	-12.70	0
$P7_{meta}$[d]	3,4-trans adduct	-1728.15616	63.02	90.86	-12.54	0

[a] The E_{el} was determined from B3LYP/6-311+G(2d,2p)//B3LYP/6-31+G(d,p) calculations; ZPE, Thermal corr. to Gibbs Free Energy, E_{disp} and NImag are from B3LYP/6-31+G(d,p) calculations.

[b] High energy transition states, associated with the formation of adducts, in which the orientation of the HCl leads to formation of *m*-substituted product;

[c] The E_{el} was determined from IEF-PCM single-point calculations on gas-phase B3LYP/6-311+G(2d,2p) optimized structure;

[d] High energy adducts, leading to *m*-substituted product formation.

Table S6. Electronic (E_{el}), thermal correction to Gibbs Free Energy, ZPE, and E_{disp} Energies as well as NImag of species involved in the catalyzed by HCl anisole-Cl_2 reaction in simulated CCl_4 solvent, computed at PBEPBE/6-311+G(2d,2p) with stable wavefunction, no diradical character.

Species	Description	E_{el} [a.u.]	Thermal corr. [a.u.]	ZPE [kcal/mol]	E_{disp} [kcal/mol]	NImag [freq cm^{-1}]
anisole		-346.43720	61.46	80.99	-3.45	0
Cl_2		-920.01680	-12.94	0.76	-0.01	0
HCl		-460.62819	-7.15	4.08	0.00	0
π-*ortho*		-1266.46376	57.61	82.30	-5.22	0
π-*para*		-1266.46294	57.63	82.25	-5.41	0
TS1	*o*-substitution	-1727.07983	59.22	85.94	-6.82	1 (*i*=115.2)
TS2	*m*-substitution	-1727.06476	58.67	85.14	-6.60	1 (*i*=255.7)
TS3	*p*-substitution	-1727.08310	59.95	86.36	-6.50	1 (*i*=82.1)
TS4	2,3-cis addition	-1727.07739	59.65	86.16	-7.03	1 (*i*=128.0)
$TS4_{meta}$[a]	2,3-trans addition	-1727.06353	57.86	85.06	-7.07	1 (*i*=86.0)
TS5	3,4-cis addition	-1727.08441	59.36	86.14	-6.90	1 (*i*=141.6)
$TS5_{meta}$[a]	3,4-cis addition	-1727.06366	58.51	85.07	-6.96	1 (*i*=425.3)
TS6	2,3-cis-trans	-1727.08065	58.92	86.04	-7.31	1 (*i*=33.5)
TS7[b]	3,4-cis-trans	-1727.08574	59.26	85.85	-7.39	1 (*i*=69.3)
$TS7_{meta}$[a]	3,4-cis-trans	-1727.06733	58.69	85.22	-7.32	1 (*i*=65.9)
TS8	2,3-cis HCl eli	-1727.09471	60.03	86.20	-7.91	1 (*i*=100.5)
$TS8_{meta}$[a]	2,3-cis HCl eli	-1727.08277	60.57	86.08	-8.23	1 (*i*=124.1)
TS9	3,4-cis HCl eli	-1727.10036	60.38	86.46	-7.70	1 (*i*=77.9)
$TS9_{meta}$[a]	3,4-cis HCl eli	-1727.08374	60.08	85.66	-7.79	1 (*i*=165.0)
TS10	cis-cis rot.	-1727.09295	60.27	87.42	-7.40	1 (*i*=93.8)
TS11	trans-trans rot.	-1727.09732	60.27	87.67	-7.49	1 (*i*=106.0)
P1	*o*-substituted	-1727.13532	56.18	85.35	-7.67	0
P2	*m*-substituted	-1727.13717	54.76	85.27	-5.80	0
P3	*p*-substituted	-1727.13673	54.66	85.30	-5.73	0
P4	2,3-cis adduct	-1727.10235	61.07	88.13	-7.36	0
P5'	3,4-cis adduct	-1727.10536	61.21	88.08	-7.74	0
$P5'_{meta}$[c]	3,4-cis adduct	-1727.10147	60.84	88.07	-7.30	0
P5''	3,4-cis adduct	-1727.09890	60.17	87.78	-7.30	0
P6	2,3-trans adduct	-1727.10854	60.98	88.32	-7.55	0
$P6_{meta}$[c]	2,3-trans adduct	-1727.10163	60.78	88.08	-8.10	0
P7'	3,4-trans adduct	-1727.10933	60.63	88.28	-7.38	0
$P7'_{meta}$[c]	3,4-trans adduct	-1727.10812	61.39	88.34	-7.40	0
P7''	3,4-trans adduct	-1727.10323	60.57	88.07	-7.38	0

[a] High energy transition states, associated with the formation of adducts, in which the orientation of the HCl leads to formation of *m*-substituted product;

[b] The E_{el} was determined from IEF-PCM single-point calculations on gas-phase PBEPBE/6-311+G(2d,2p) optimized structure; ZPE, Thermal corr. to Gibbs Free Energy, E_{disp} and NImag are from gas-phase calculations.

[c] High energy adducts, leading to m-substituted product formation.

Table S7. Electronic (E_{el}) energies of species involved in the catalyzed by HCl anisole-Cl_2 reactions in isolation (gas phase) and in simulated CCl_4 solvent, computed at RB2-PLYP/6-311+G(2d,2p)//RB3LYP/6-311+G(2d,2p).

gas phase			CCl_4 solvent		
Species	Description	E_{el} [a.u.]	Species	Description	E_{el} [a.u.]
π-*ortho*		-1266.65825	**π-*ortho***		-1266.66059
π-*para*		-1266.65819	**π-*para***		-1266.66049
TS1	*o*-substitution	-1727.29579	**TS1**	*o*-substitution	-1727.31867
TS2	*m*-substitution	-1727.28106	**TS2**	*m*-substitution	-1727.29904
TS3	*p*-substitution	-1727.29812	**TS3**[a]	*p*-substitution	-1727.32191
TS4	2,3-cis addition	-1727.29551	**TS4**	2,3-trans addition	-1727.31960
$TS4_{meta}$[b]	2,3-cis addition	-1727.28440	**$TS4_{meta}$**[b]	2,3-trans addition	-1727.30196
TS5	3,4-cis addition	-1727.30007	**TS5**	3,4-cis addition	-1727.32596
$TS5_{meta}$[b]	3,4-cis addition	-1727.28150	**$TS5_{meta}$**[b]	3,4-cis addition	-1727.29942
TS6	2,3-cis-trans isomerization	-1727.30165	**TS7**	3,4-cis-trans isomerization	-1727.33170
TS7	3,4-cis-trans isomerization	-1727.30881	**$TS7_{meta}$**[b]	3,4-cis-trans isomerization	-1727.30847
$TS7_{meta}$[b]	3,4-cis-trans isomerization	-1727.29020	**TS8**	2,3-cis HCl elimination	-1727.33568
TS8	2,3-cis HCl elimination	-1727.32144	**$TS8_{meta}$**[b]	2,3-cis HCl elimination	-1727.32086
$TS8_{meta}$[b]	2,3-trans HCl elimination	-1727.29121	**TS9**	3,4-cis HCl elimination	-1727.34307
TS9	3,4-cis HCl elimination	-1727.32844	**$TS9_{meta}$**[b]	3,4-cis HCl elimination	-1727.32075
$TS9_{meta}$[b]	3,4-cis HCl elimination	-1727.31126	**TS10**	cis-cis rotation	-1727.34426
TS11	trans-trans rotation	-1727.34505	**TS11**	trans-trans rotation	-1727.34842
P1	*o*-product	-1727.38459	P1	*o*-product	-1727.38735
P2	*m*-product	-1727.38684	P2	*m*-product	-1727.38921
P3	*p*-product	-1727.38642	P3	*p*-product	-1727.38884
P4	2,3-cis adduct	-1727.34737	P5'	3,4-cis adduct	-1727.35421
P5''	3,4-cis adduct	-1727.34316	$P5_{meta}$[c]	3,4-cis adduct	-1727.35180
$P5_{meta}$[c]	3,4-cis adduct	-1727.34798	P5''	3,4-cis adduct	-1727.34746
P6	2,3-trans adduct	-1727.35437	P6	2,3-trans adduct	-1727.35775
P7'	3,4-trans adduct	-1727.35573	$P6_{meta}$[c]	2,3-trans adduct	-1727.35058
P7''	3,4-trans adduct	-1727.34746	P7'	3,4-trans adduct	-1727.35884
$P7_{meta}$[c]	3,4-trans adduct	-1727.35445	P7''	3,4-trans adduct	-1727.35150
			$P7_{meta}$[c]	3,4-trans adduct	-1727.35789

[a] B2-PLYP/6-311+G(2d,2p)//B3LYP/6-31+G(d,p);

[b] High energy transition states, associated with the formation of adducts, in which the orientation of the HCl leads to formation of *m*-substituted product;

[c] High energy adducts, leading to *m*-substituted product formation.

Table S8. Cartesian coordinates species involved in HCl-catalyzed anisole-Cl_2 reactions in isolation (gas-phase) at RB3LYP/6-311+G(2d,2p). The energy data for these structures are shown in Table S4.

anisole
C,0,-0.922113,-0.519093,0.
C,0,0.,0.527366,0.
C,0,1.369741,0.246632,0.
C,0,1.80792,-1.067384,0.
C,0,0.893257,-2.120843,0.
C,0,-0.464811,-1.836836,0.
H,0,-1.98344,-0.325516,0.
H,0,2.067374,1.072118,0.
H,0,2.869976,-1.272255,0.
H,0,1.238352,-3.144984,0.
H,0,-1.186483,-2.64264,0.
O,0,-0.333755,1.851301,0.
C,0,-1.710443,2.199139,0.
H,0,-2.216943,1.822151,0.891537
H,0,-1.743156,3.28468,0.
H,0,-2.216943,1.822151,-0.891537

Cl_2
Cl,0,-1.0178691818,0.,0.
Cl,0,1.0178691818,0.,0.

HCl
Cl,0,0.,0.,0.0711080502
H,0,0.,0.,-1.2088368529

anisole-Cl_2 pi-complex ortho
C,0,1.2376330032,0.1508828686,1.092028594
C,0,1.6667432259,0.9307106369,0.0075926579
C,0,2.2919449744,0.3183581882,-1.0786929495
C,0,2.4937898789,-1.0605637031,-1.0658516007
C,0,2.0810528463,-1.8378562019,0.0089991813
C,0,1.4527444085,-1.2229866771,1.0880973502
H,0,0.7817497189,0.6461478156,1.93705175
H,0,2.62372077,0.8964395129,-1.9267357856
H,0,2.2430624211,-2.9060078605,0.0058444174
H,0,1.1236037253,-1.8113822917,1.9333954456
Cl,0,-3.51573735,-0.1376369902,-0.3805505633
Cl,0,-1.5246145994,-0.1159167874,0.1710972526
H,0,2.9800337681,-1.5259603508,-1.9125804218
O,0,1.4353892421,2.2654416668,0.114660519
C,0,1.7972823373,3.1072935108,-0.9730642192
H,0,1.2647039572,2.8271928251,-1.8840767329
H,0,1.5064262463,4.111147757,-0.6791566012
H,0,2.8737582956,3.0802797907,-1.1547833738

anisole-Cl_2 pi-complex para
C,0,-0.6543728517,1.6477532357,-0.0516614019
C,0,-1.0637194425,1.1540337479,1.1841623427
C,0,-1.9830143941,0.1124425277,1.2696835888
C,0,-2.5039714466,-0.4409332862,0.0984973816
C,0,-2.1016636906,0.0550124995,-1.1482023115
C,0,-1.1872228886,1.0884390574,-1.2187855132
H,0,0.0310179413,2.4806977943,-0.107960357
H,0,-0.6644739123,1.580765378,2.0939173301
H,0,-2.279666419,-0.2562939308,2.2388699409
H,0,-2.5180834842,-0.390408803,-2.0402449702
H,0,-0.8814734539,1.4646908668,-2.1852114949
Cl,0,3.7164941218,-0.7472783372,0.0674569388
Cl,0,1.8680853202,0.1847460849,0.0507718321
O,0,-3.4022807694,-1.460852638,0.0632357811
C,0,-3.8409658941,-2.024592384,1.2932383088
H,0,-4.356702998,-1.2839609278,1.9079648042
H,0,-4.5342591878,-2.8159095323,1.0250635021
H,0,-3.0060115308,-2.4485890229,1.8546397673

TS1
C,0,-2.910097,0.374467,-0.21787
C,0,-2.601603,-2.034999,0.178656
C,0,-3.401119,-0.917193,-0.166648
C,0,-1.286608,-1.8535,0.460448
C,0,-1.568182,0.600331,0.095345
C,0,-0.663092,-0.527584,0.399772
Cl,0,0.535782,-0.626298,-1.029057
H,0,-3.563932,1.190842,-0.479325
H,0,-3.044063,-3.019543,0.202318
H,0,-0.635903,-2.678127,0.713271
H,0,0.039499,-0.302621,1.219325
Cl,0,3.469452,-0.037171,-1.111661
H,0,2.90779,0.038203,0.412815
Cl,0,2.288237,0.088881,1.820097
H,0,-4.444593,-1.079501,-0.403225
O,0,-0.990697,1.76781,0.16284
C,0,-1.698788,2.970435,-0.196576
H,0,-0.972797,3.76617,-0.081195
H,0,-2.032112,2.912048,-1.231017
H,0,-2.540397,3.126314,0.4761

TS2
C,0,-2.046102508,1.6500271751,-1.228142864
C,0,-2.3693866917,-0.225729546,0.3341739136
C,0,-2.8696087161,0.7296573233,-0.585980425
C,0,-1.0263006722,-0.2511348708,0.6042782178
C,0,-0.6954106074,1.6522070477,-0.9661566963
C,0,-0.1250665019,0.698787967,-0.0334275396
Cl,0,1.0834110238,-0.2840126368,-1.1213423734
H,0,-2.4728934918,2.3479113948,-1.9333363752
H,0,-0.5788370388,-0.9529401357,1.2904656938
H,0,-0.0249090157,2.3464784289,-1.4506090666
H,0,0.6253364111,1.0958779702,0.6803087229
Cl,0,3.8030402375,-1.2383166802,-0.5590457899
H,0,3.2466687335,-0.3636979229,0.6389855481
Cl,0,2.5857825452,0.5145226641,1.771659856
H,0,-3.9322031628,0.712249899,-0.7894383497
O,0,-3.3036273179,-1.0440749663,0.8609921994
C,0,-2.8709329322,-2.0501431792,1.7838280549
H,0,-3.768590304,-2.5850841488,2.0736443509
H,0,-2.1693056431,-2.7362129798,1.307971138
H,0,-2.4109903478,-1.5974408037,2.6632617842

TS3
C,0,-0.6918134881,3.9386063614,1.2611134741
C,0,-0.291991195,4.1453061287,-1.1742078955
C,0,-0.4275335905,4.7328477487,0.1136387208
C,0,-0.4134306242,2.8039634921,-1.3173752534
C,0,-0.8168878869,2.5932261903,1.1182795652
C,0,-0.6777664122,1.9285627514,-0.17562791
Cl,0,0.8120105748,0.795914183,0.001872445
H,0,-0.7829483776,4.3943585368,2.2338290816
H,0,-0.0814309911,4.7970614489,-2.0091587293
H,0,-0.3045289197,2.3364198275,-2.2856022942
H,0,-1.0163032088,1.9603900085,1.9717792249
H,0,-1.449289229,1.1609008287,-0.3475143503
Cl,0,1.0612300668,-2.1549795577,0.172510568
H,0,-0.5288878355,-1.6975489415,0.0414839097
Cl,0,-1.9458357935,-1.1831947766,-0.0782411404
O,0,-0.2778784902,6.0416141206,0.147642202
C,0,-0.3802209378,6.7676083088,1.3902323057
H,0,0.3887265229,6.4368287016,2.0854859921
H,0,-0.2191547162,7.8053540962,1.1230297043
H,0,-1.3715939152,6.6421193598,1.8211029168

TS4

C,0,-2.2684745066,-1.4344137795,0.0063036174
C,0,-2.8507091743,0.7397375073,-0.8006645106
C,0,-2.9935799982,-0.6430663198,-0.8708387484
C,0,-1.9952549775,1.3908070331,0.1096323873
C,0,-1.262178903,-0.8248171998,0.9056521261
C,0,-1.2307880595,0.6510314865,0.9564061316
H,0,-3.4355651644,1.3445654785,-1.481695083
H,0,-3.6784491066,-1.07706579,-1.580980137
H,0,-1.9168749309,2.4667649914,0.1052516775
H,0,-1.2446939203,-1.2998035617,1.8825886425
H,0,-0.5361664175,1.1125599821,1.6411973992
Cl,0,1.5602656683,2.0176319678,0.2533981262
H,0,2.4179708287,0.6798014034,-0.2523575241
Cl,0,0.4000924999,-1.2629243887,0.1503393988
Cl,0,3.1079274929,-0.582573962,-0.6912792923
O,0,-2.3707940759,-2.7380878747,0.1310717911
C,0,-3.19000096,-3.4894628461,-0.7855273831
H,0,-2.8422736758,-3.3382790464,-1.8057381979
H,0,-3.0613100544,-4.5258032143,-0.4965808003
H,0,-4.2342894568,-3.1981555791,-0.684841567

TS4(meta)

C,0,0.7870946646,2.4837266893,-0.221180141
C,0,2.4617926703,0.8197419061,-0.6021961725
C,0,1.8965973,2.0644884808,-0.9012514495
C,0,1.9352260422,-0.0529763249,0.3761939192
C,0,0.1569182444,1.6044805609,0.7603577624
C,0,0.8021837863,0.323143943,1.0635235701
H,0,0.3214944363,3.4373129178,-0.4188452831
H,0,3.3460484736,0.4873241856,-1.1301423896
H,0,2.3443283464,2.6818303898,-1.6658943379
H,0,-0.1984887776,2.1175100174,1.6509951895
H,0,0.3400705187,-0.3079622996,1.8047551371
Cl,0,-1.3673393604,-2.0685016286,0.7989796627
H,0,-2.6833916526,-1.2880308337,-0.03367263
Cl,0,-1.4904946721,1.2088602574,-0.1215733754
Cl,0,-3.6982030095,-0.5134640033,-0.722164754
O,0,2.625981496,-1.1905264095,0.5433165759
C,0,2.1753660494,-2.1338770043,1.5356653578
H,0,2.2356335401,-1.6881401611,2.5300354348
H,0,1.159302888,-2.4597066692,1.3219028563
H,0,2.8664006151,-2.966787327,1.4672111174

TS5

C,0,-2.2126516915,-1.42156311,0.0148421422
C,0,-2.8737502408,0.7147824628,-0.8539012501
C,0,-2.9606949773,-0.7108161988,-0.861501974
C,0,-2.0323817131,1.4013171946,0.0558584643
C,0,-1.266501808,-0.7734987768,0.9291562875
C,0,-1.2540534583,0.7011806692,0.9138325307
H,0,-2.2578762208,-2.5011728992,0.0294974758
H,0,-3.6089574323,-1.214047444,-1.5604323708
H,0,-1.9883303612,2.4784410884,0.003618876
H,0,-1.3075852457,-1.1791546367,1.9383956814
H,0,-0.5731287935,1.209166083,1.5792145711
Cl,0,1.5327479736,1.9927753599,0.0424584179
H,0,2.4138410638,0.6533667054,-0.2286925931
Cl,0,0.4342166897,-1.306374889,0.3310599425
Cl,0,3.1625564106,-0.6659292125,-0.4621501178
O,0,-3.5530626333,1.4830313171,-1.6770560183
C,0,-4.4130700337,0.9213714371,-2.6898929118
H,0,-3.8374967542,0.2938404429,-3.3670916157
H,0,-5.2226158784,0.3578577431,-2.2301075477
H,0,-4.8114496785,1.7761698447,-3.2235742063

TS5(meta)

C,0,-2.16824882,-1.4461166298,0.0149359833
C,0,-2.83987654,0.7099608598,-0.8170010522
C,0,-2.9200881694,-0.7087299969,-0.8560445103
C,0,-2.0150095828,1.3908505251,0.0666723682
C,0,-1.2496071884,-0.7797611567,0.9340246977
C,0,-1.2213602111,0.6831765415,0.9411754516
H,0,-2.1847074261,-2.5237653484,0.0251350674
H,0,-3.4513474056,1.2561703609,-1.5230915728
H,0,-1.9715299111,2.4689097785,0.0457370435
H,0,-1.2685520457,-1.1958397468,1.9402982902
H,0,-0.577196718,1.1825471186,1.6462168806
Cl,0,1.4053766946,1.9275289148,-0.0916439748
H,0,2.3619791937,0.627754585,-0.2533976153
Cl,0,0.5287421155,-1.2794419592,0.4059365367
Cl,0,3.1637748194,-0.6845116957,-0.3715492918
O,0,-3.7699383198,-1.1926512854,-1.7883259157
C,0,-3.8742452187,-2.6106375262,-1.9284694894
H,0,-2.9081534484,-3.0466813403,-2.1867131676
H,0,-4.2559565843,-3.065492125,-1.0125245816
H,0,-4.5780268138,-2.7748974736,-2.7372052657

TS6

C,0,-2.0436223063,0.9127636478,-0.3811838016
C,0,-1.3569112767,-1.2975022578,0.2403731716
C,0,-2.377630104,-0.3716306077,-0.0204747662
C,0,0.0105328258,-0.9960274952,0.1694309039
C,0,-0.601924516,1.3119279901,-0.497943045
C,0,0.3998684722,0.2631297851,-0.1726895845
H,0,-1.6493820708,-2.3028932254,0.5155209441
H,0,0.7609507713,-1.7337668255,0.4062713473
H,0,-0.4213863178,1.6546471228,-1.5211193929
H,0,1.4422217206,0.5315631889,-0.2279525407
Cl,0,3.0425963575,-0.4089446818,1.5038917204
H,0,3.2323023998,-0.7422155875,-0.181368124
Cl,0,-0.2794348846,2.764141367,0.5499192454
Cl,0,3.1800224198,-0.9503531465,-1.6150326511
H,0,-3.4080093533,-0.6778465724,0.061875982
O,0,-2.8823461519,1.8780574182,-0.683866418
C,0,-4.3020887169,1.6481786609,-0.6016380108
H,0,-4.5986511113,0.870095716,-1.3032384724
H,0,-4.5788702779,1.376047843,0.4154152826
H,0,-4.7586898225,2.592364248,-0.8738030351

TS7

C,0,-2.0004411603,0.9042068647,-0.569405514
C,0,-1.3513701395,-1.3153987939,0.0988928978
C,0,-2.3649320505,-0.3450536142,-0.2325268488
C,0,0.0185212889,-0.9811102805,0.1089447143
C,0,-0.5736242333,1.2993389381,-0.6478398232
C,0,0.4087784259,0.2745360584,-0.2187265045
H,0,-2.7396479495,1.6572739372,-0.80260076
H,0,0.7495729245,-1.7166527262,0.4087702458
H,0,-0.3380953602,1.5694891425,-1.6839280753
H,0,1.4550198218,0.5365320136,-0.2001086507
Cl,0,2.8758584209,-0.3802794166,1.724289051
H,0,3.2249464024,-0.8143179134,0.0894512804
Cl,0,-0.3283409776,2.8490025025,0.2822786069
Cl,0,3.3173559557,-1.118763982,-1.3265122994
H,0,-3.4077209179,-0.6174261604,-0.1963452915
O,0,-1.6345984429,-2.5536136136,0.4237162043
C,0,-2.9927489314,-3.0390543837,0.4774264691
H,0,-3.5573511282,-2.4986556213,1.2342656654
H,0,-3.4652913842,-2.9532905276,-0.4989366336
H,0,-2.9032071816,-4.0822607543,0.7561532179

TS7(meta)

C,0,-1.9432587148,1.0420658558,-0.4667347174
C,0,-1.3460087189,-1.2389680154,0.0537602586
C,0,-2.3333745196,-0.2335705505,-0.2095326903
C,0,0.0094744751,-0.9771016842,0.0867211952
C,0,-0.5010645334,1.3630511431,-0.5251678201
C,0,0.4579659663,0.308989336,-0.1455966576
H,0,-2.6386126848,1.8406796693,-0.6662395491
H,0,-1.712086812,-2.2387590247,0.2482934118
H,0,0.7254226588,-1.7476843721,0.3236822303
H,0,-0.2430711486,1.5853410934,-1.5740919262
H,0,1.5046315266,0.5540894766,-0.0979564625
Cl,0,2.9041642521,-0.5486593363,1.6791924212
H,0,3.1381826999,-0.8201728876,0.0652610135
Cl,0,-0.1277641395,2.920927903,0.3425291264
Cl,0,3.1115624814,-0.9739968139,-1.4248328296
O,0,-3.6001513073,-0.6918848071,-0.1575245256
C,0,-4.660658439,0.2425839022,-0.3706723505
H,0,-4.6376889208,1.0314687082,0.3826437091
H,0,-4.597974786,0.6778418982,-1.3694165645
H,0,-5.5781309903,-0.3278832755,-0.2769925818

TS8

C,0,1.8069810365,-0.7722487605,-1.2250474731
C,0,2.0595911054,0.2461457696,-0.3008847018
C,0,1.035625094,1.099192692,0.0590568652
C,0,-0.3426201559,0.8760518867,-0.4551019377
C,0,-0.513185638,-0.2378261617,-1.4063199684
C,0,0.5479599396,-1.0183587729,-1.7779993886
Cl,0,-1.0563465149,2.3977105572,-1.1465291793
H,0,2.6367997593,-1.398561352,-1.5262485205
H,0,-0.9671082727,0.6745801445,0.4595388272
H,0,-1.4852247106,-0.3459637675,-1.8571339361
H,0,0.4098232544,-1.8302290105,-2.474830322
Cl,0,-2.0151528465,0.1830894726,2.2296318603
Cl,0,-1.9078841784,-2.1711814607,0.1812282356
H,0,-2.025851276,-1.0236742491,1.3102647883
H,0,3.0538385199,0.3719571705,0.0960102617
O,0,1.131937681,2.1067028156,0.8938873224
C,0,2.3714702336,2.3602335769,1.5776054452
H,0,2.6527167826,1.4958993785,2.1767740215
H,0,3.1547116556,2.6059249849,0.8618152174
H,0,2.172077609,3.210436651,2.2191715056

TS8(meta)
C,0,1.5743268343,-0.4840561903,-0.1980570249
C,0,2.3333453872,1.8746479781,-0.2875223856
C,0,2.5890913326,0.4888203063,-0.2421614865
C,0,1.053241136,2.3254139523,-0.3052812764
C,0,0.2553621011,-0.0729822265,-0.2499415389
C,0,-0.0728070549,1.3713099323,-0.2848006776
H,0,3.1656517486,2.5630327025,-0.2999665869
H,0,0.814684297,3.3783688542,-0.3005327356
H,0,-0.5696984843,-0.7674280053,-0.2940673283
H,0,-0.7644738781,1.5419393207,-1.1175025421
Cl,0,-2.0102750963,-1.64948742741,1.3150308092
H,0,-2.7968445268,-0.8586727745,-0.2562837246
Cl,0,-1.0594388952,1.8391034863,1.1916581245
Cl,0,-3.136118325,-0.2387965852,-1.4286296239
H,0,3.6111055278,0.1323679527,-0.2576251307
O,0,2.003149161,-1.7528861949,-0.1534033912
C,0,1.0281581828,-2.8173706898,-0.2319927722
H,0,0.5312061189,-2.7946267315,-1.2022240328
H,0,1.6033238403,-3.7311138337,-0.1326039897
H,0,0.2903926342,-2.7324846473,0.5630764202

TS9
C,0,1.7866886487,-0.8011612238,-1.2180023236
C,0,2.0323777412,0.2142707243,-0.2341154645
C,0,1.0308505402,1.0199308909,0.1605077627
C,0,-0.3422961841,0.8282958019,-0.3330366983
C,0,-0.5157023266,-0.1799169011,-1.3868102694
C,0,0.5226147958,-0.965357531,-1.8042277322
Cl,0,-1.1008397104,2.4121067066,-0.8179989248
H,0,1.1899849862,1.7922179266,0.8989441619
H,0,-0.9626675157,0.5051176286,0.5557005016
H,0,-1.4821730446,-0.2508081509,-1.8571436394
H,0,0.3494957383,-1.7229874398,-2.5499790338
Cl,0,-2.1093545724,-0.2141520321,2.1713346797
Cl,0,-2.0464341252,-2.3190467748,-0.1421580121
H,0,-2.1379978136,-1.2943927275,1.116364058
H,0,3.0330964129,0.2996657419,0.1627538795
O,0,2.8411050012,-1.5346672391,-1.5139972181
C,0,2.7302958912,-2.6289602395,-2.4481888849
H,0,1.9852700987,-3.3427049757,-2.1029232568
H,0,2.4780902375,-2.2552776091,-3.4387535926
H,0,3.7121084297,-3.0874998354,-2.4619034709

TS9(meta)
C,0,1.4709324099,-1.695269549,-0.6804633271
C,0,1.9953832621,-0.5746878921,0.0353513009
C,0,1.2986279308,0.5932315076,0.0602218333
C,0,-0.0303302679,0.6646189278,-0.5585893983
C,0,-0.5005232731,-0.4913743097,-1.3092920353
C,0,0.2603863067,-1.6570042871,-1.3288248364
Cl,0,-0.3045983774,2.220125632,-1.4627473656
H,0,1.6420643751,1.4670856703,0.588992488
H,0,-0.7585862126,0.7761623126,0.3226578159
H,0,-1.3698967323,-0.3803046616,-1.9337504895
H,0,-0.100123548,-2.5218022189,-1.8643864964
Cl,0,-2.1093868981,0.9143716307,1.8347310411
Cl,0,-2.6402571591,-1.5997686335,0.0643546536
H,0,-2.4585103204,-0.3207680169,1.0644405519
H,0,2.0766627084,-2.5913147109,-0.7021520557
O,0,3.192343372,-0.8074066838,0.6198720463
C,0,3.7934078341,0.2595801864,1.3545831191
H,0,4.7257785371,-0.1376723673,1.7411855176
H,0,3.99801503,1.1121435603,0.7045852986
H,0,3.1532410229,0.568804903,2.1823753381

TS11
C,0,-0.9831713783,1.5470501103,0.3495990784
C,0,-2.0458872169,0.9571956344,1.156469384
C,0,-2.2677979525,-0.361249802,1.1525485237
C,0,-1.4445112973,-1.2612193451,0.3014654783
C,0,-0.0938109531,-0.6807740277,-0.1039649924
C,0,-0.056522734,0.7876726792,-0.2538029945
Cl,0,-2.3928622355,-1.6132037064,-1.2615765436
H,0,-3.0687701412,-0.8034109523,1.7268930099
H,0,-1.3169044012,-2.2434778721,0.7388682969
H,0,0.3034230902,-1.2049394463,-0.9638253408
H,0,0.7578773978,1.2333033981,-0.8053704801
Cl,0,3.9493017092,-0.6668545597,-1.0202274441
Cl,0,1.1316160529,-1.1830680769,1.2573056713
H,0,3.0741352452,-0.8830676395,-0.0944461749
H,0,-2.6500815044,1.6307762695,1.7479051728
O,0,-0.9477140401,2.9169068402,0.2997985501
C,0,-1.4729596885,3.5054441847,-0.8967347324
H,0,-1.3681011823,4.5797285026,-0.7762842044
H,0,-0.911018483,3.1775449462,-1.772420674
H,0,-2.5274914701,3.2520377185,-1.0254631263

P1
C,0,-2.0549671401,0.5197086515,0.4308829919
C,0,-2.3012230615,-1.8842463743,0.3893321235
C,0,-2.4116893601,-0.6712440262,1.0591544939
C,0,-1.8360450814,-1.8997646049,-0.9255399784
C,0,-1.5862802703,0.514303564,-0.8846644982
C,0,-1.4846036591,-0.7185333533,-1.5540494358
Cl,0,-0.9009935816,-0.7561900212,-3.2010207048
H,0,-2.1361837087,1.4495974994,0.9705454322
H,0,-2.5865691484,-2.8088471416,0.8702242871
H,0,-1.7451291336,-2.8291962801,-1.4676820562
H,0,-0.0752996353,-1.5645299783,1.3750514492
Cl,0,1.1640139642,2.0893148291,2.6088164514
H,0,1.1791588104,0.8276011506,2.3386940924
Cl,0,1.1272418727,-1.5776316058,1.8506698129
H,0,-2.7783713922,-0.6420134456,2.0758009462
O,0,-1.2159535848,1.6160037236,-1.5709947844
C,0,-1.2811675269,2.8823431277,-0.9181551903
H,0,-0.9264030419,3.6026564126,-1.6483037883
H,0,-2.306998439,3.1259708671,-0.6354958356
H,0,-0.637362625,2.9056742528,-0.0379530532

P2
C,0,1.6277827152,0.8274351477,0.2314592309
C,0,2.8191198553,-1.1465089842,0.9284013354
C,0,2.5946429514,0.214292663,1.0369243819
C,0,2.0992106722,-1.9300614649,0.0253804737
C,0,0.8851686066,0.0592402269,-0.6708258378
C,0,1.1449131532,-1.30851108,-0.7605911912
H,0,3.5669860169,-1.6137709698,1.5537792247
H,0,2.2764362907,-2.9903708013,-0.0626743821
H,0,0.1402747073,0.5005129963,-1.3122099574
H,0,-0.5657643595,-0.7521776515,1.1899188269
Cl,0,-3.4607135724,1.876214878,0.6649459296
H,0,-2.873822831,0.8693783797,1.2179388429
Cl,0,0.2226143417,-2.2593843068,-1.9153173515
Cl,0,-1.4801403189,-0.9466813927,2.08015472
H,0,3.1528504386,0.8240961909,1.7318121254
O,0,1.4790583857,2.1647544228,0.3924139674
C,0,0.5384559009,2.856251592,-0.4276320391
H,0,-0.4790283134,2.5052654625,-0.2495402786
H,0,0.6130441922,3.9002684494,-0.1406820793
H,0,0.7882711672,2.750966242,-1.4850459419

P3
C,0,-1.5741111744,-0.5075818379,-0.6830084159
C,0,-2.3925741655,-0.4609434217,1.5866063303
C,0,-2.5266112373,-0.0850017942,0.2447093404
C,0,-1.3286379894,-1.244605565,1.996294395
C,0,-0.5015631148,-1.2999046596,-0.2682600358
C,0,-0.3825538201,-1.6640420555,1.0639330825
Cl,0,0.9635008915,-2.6687887952,1.5802077306
H,0,-1.6460180902,-0.2314740158,-1.7230408338
H,0,-3.1345184262,-0.1243589283,2.2962003641
H,0,-1.2298030115,-1.5312633082,3.0325126911
H,0,0.2280573409,-1.6380736787,-0.9894465415
H,0,0.67009889,0.7481665721,0.4507871051
Cl,0,-0.1575018428,3.0888151953,-2.6545050309
H,0,0.3959546318,2.7227435823,-1.5474678652
Cl,0,1.3337179327,1.8521407112,0.5331941547
O,0,-3.6045234379,0.685601241,-0.050310246
C,0,-3.7862123268,1.1119532401,-1.3983804513
H,0,-3.9196596145,0.2584952648,-2.0663490688
H,0,-4.6901809403,1.7128436149,-1.3966317557
H,0,-2.9457547779,1.7189594361,-1.7384083605

P4
C,0,-2.2249284213,-0.1888801809,0.1343966724
C,0,-1.3445249255,1.9534642474,-0.5767541638
C,0,-2.3501256204,0.9116516039,-0.6373253434
C,0,-0.1581701362,1.7814230797,0.0297651576
C,0,-1.0958633452,-0.2251652885,1.1412472666
C,0,0.1639198094,0.4703740848,0.6464315132
H,0,-1.558803064,2.8897201273,-1.0747331786
H,0,-3.1943055124,1.0411368597,-1.2955903791
H,0,0.61115512,2.5384328908,0.0049561455
H,0,-1.4223250418,0.3689576989,2.0001298569
H,0,0.8881522328,0.5325710657,1.4490959363
Cl,0,1.0640339023,-0.5928310681,-0.628540389
H,0,2.9975971371,0.740420637,-0.7568043169
Cl,0,-0.7658050729,-1.8584941071,1.8243672015
Cl,0,3.9795671532,1.5818564209,-0.6939740602
O,0,-3.0616068616,-1.2312870562,0.2004452961
C,0,-4.1935429756,-1.2338938105,-0.667877025
H,0,-3.8780727531,-1.1915415449,-1.7112176736
H,0,-4.7097908935,-2.1683826593,-0.4749849564
H,0,-4.8527510776,-0.392812087,-0.4462933451

P4(meta)

C,0,-1.4276975871,-2.4970544769,0.0472829425
C,0,-2.888230769,-0.6626538887,-0.6051456237
C,0,-2.5230991296,-2.0662387639,-0.5913510278
C,0,-2.0171168682,0.2908452984,-0.2186884324
C,0,-0.6591162895,-1.4949865446,0.8457806758
C,0,-0.6432796396,-0.097211052,0.2382399753
H,0,-1.1329201797,-3.5337859124,0.0808145845
H,0,-3.8482326362,-0.3592477302,-0.9972838412
H,0,-3.164159923,-2.7664235005,-1.1089800174
H,0,-1.1635499726,-1.3630964759,1.8096021893
H,0,-0.2091299853,0.5976567838,0.9457453975
Cl,0,0.4979574211,0.0319789681,-1.2402592377
H,0,2.1096516083,1.4632735295,-0.2475296476
Cl,0,0.9998372695,-2.0655224856,1.2940532847
Cl,0,2.7189931994,2.3733597036,0.4402743246
O,0,-2.3375327011,1.5950179458,-0.4032202569
C,0,-1.6449704845,2.6074924108,0.332216836
H,0,-1.7132097388,2.4290614075,1.4072216685
H,0,-0.6014288702,2.6844855089,0.0291204978
H,0,-2.153350406,3.5360282709,0.0922488503

P5''

C,0,-1.4533888091,-1.9237190818,-0.2024544441
C,0,-2.2717957892,0.3586785296,-0.1129591603
C,0,-2.3739029209,-1.0272994156,-0.5699716167
C,0,-1.1309553193,0.8182171654,0.4446879647
C,0,-0.3781748081,-1.5114778195,0.7534989601
C,0,0.0459454266,-0.0621352512,0.5770677181
H,0,-1.4896606088,-2.9505497855,-0.5330430682
H,0,-3.1813438032,-1.3178304514,-1.2241191603
H,0,-1.0330680372,1.8647965992,0.6903244381
H,0,-0.7872013577,-1.5605164985,1.76759398
H,0,0.7131525714,0.237732541,1.3753914264
Cl,0,1.1610606052,0.1456146381,-0.9543633115
H,0,2.864955814,1.2915946766,0.1495419805
Cl,0,1.0039852043,-2.6786407915,0.7776643482
Cl,0,3.6594518031,1.9407963583,0.9404451603
O,0,-3.2906384374,1.2364490025,-0.291230657
C,0,-4.577302973,0.7617327687,-0.68615887
H,0,-4.5737867601,0.4082801917,-1.7182342601
H,0,-4.9321167827,-0.0286180689,-0.0234279594
H,0,-5.2383700381,1.6193764682,-0.6087945132

P5(meta)

C,0,-1.573324435,-0.5134310991,0.5875514472
C,0,-2.2589052859,1.7160980259,-0.1230778041
C,0,-2.4214990707,0.2633492842,-0.1077882088
C,0,-1.137670006,2.2937786834,0.319037129
C,0,-0.531769753,0.1647794511,1.4236489237
C,0,-0.0041524204,1.4654830722,0.8327359135
H,0,-1.6591504607,-1.5847878897,0.6473259415
H,0,-3.0632172266,2.2990210514,-0.5493952687
H,0,-0.987386773,3.3606941778,0.2406983008
H,0,-0.9610373057,0.4488998659,2.3891961049
H,0,0.6003188561,1.9893264273,1.5635938788
Cl,0,1.1759621141,1.2027381166,-0.5801143555
H,0,2.3133079349,-1.2152869974,-0.6520907778
Cl,0,0.8052488173,-0.977755309,1.8868581906
Cl,0,3.0343133222,-2.1154293157,-1.2237957883
O,0,-3.480066719,-0.1507321532,-0.8468675107
C,0,-3.7135453453,-1.5535084711,-0.9268122479
H,0,-2.8567122987,-2.0650043443,-1.3690337167
H,0,-3.9180425033,-1.9704832194,0.0614934566
H,0,-4.5836734616,-1.6763332152,-1.5636770837

P6

C,0,2.0074254429,-0.3111584044,0.1332086594
C,0,0.6817011961,-1.5627832676,-1.4624328026
C,0,1.8903150358,-1.3775576078,-0.6819018977
C,0,-0.4285211755,-0.8366385851,-1.262326057
C,0,0.9222405514,0.7134118882,0.2033542953
C,0,-0.449794119,0.19000513,-0.1995401702
H,0,0.6874378696,-2.3337208458,-2.2211554794
H,0,-1.3323171299,-1.0073876826,-1.827011962
H,0,0.8945616851,1.1835813641,1.1783315132
H,0,-1.1217081605,1.0137883417,-0.4030605143
Cl,0,-4.6311561008,-0.4121744989,0.0839254983
H,0,-3.4707972209,-0.5243262206,0.6419972959
Cl,0,1.3504570816,2.0908895176,-0.9542155655
Cl,0,-1.206814211,-0.5638709792,1.3708762128
H,0,2.6863156542,-2.0983014599,-0.7813610524
O,0,3.050056955,0.0110352576,0.9214638113
C,0,4.1936687463,-0.8406960388,0.8951199601
H,0,3.9335294995,-1.848129803,1.224269666
H,0,4.6226884737,-0.878947303,-0.1074789946
H,0,4.906949926,-0.4012088023,1.5845075835

P7'

C,0,-1.8737074716,-0.1794468065,0.3119355108
C,0,-1.7425646064,-1.1941908041,1.3530042766
C,0,-0.6519557506,-1.9580398002,1.4405109259
C,0,0.4641198056,-1.8010840236,0.4701132338
C,0,0.4786532528,-0.4603983126,-0.2510562688
C,0,-0.8315352714,0.1619937136,-0.4753411588
Cl,0,0.3048622473,-3.1329108261,-0.8185952717
H,0,-0.5654947102,-2.7336127948,2.1872830149
H,0,1.4299311847,-2.0039339485,0.9152020472
H,0,1.0896216968,-0.5093498143,-1.1422230241
H,0,-0.9032351985,0.929644315,-1.2277821393
Cl,0,0.8046073857,3.8077981195,-0.8916115201
Cl,0,1.5596690941,0.694758507,0.8542542241
H,0,1.1334069692,2.7525915699,-0.2171226934
H,0,-2.5754715779,-1.3124462591,2.0313222953
O,0,-3.1172195683,0.3389716184,0.2546582404
C,0,-3.3740657773,1.3582847158,-0.711866411
H,0,-2.7297715293,2.2221752668,-0.5445172025
H,0,-3.2246910008,0.9770629414,-1.7232473499
H,0,-4.412989174,1.6397826225,-0.5753407293

P7''

C,0,-1.9133905805,1.0791918387,-1.1232154983
C,0,-1.7212064424,-1.007263166,0.1197388
C,0,-2.4273173079,-0.110076861,-0.7915493945
C,0,-0.4460931326,-0.7598296597,0.4843425674
C,0,-0.6115933577,1.5314326468,-0.5659413306
C,0,0.266173627,0.3984798435,-0.0552762381
H,0,-2.4439419107,1.754745969,-1.7782023061
H,0,0.076695635,-1.4476018833,1.1311879057
H,0,-0.0633379264,2.1589258093,-1.2568390875
H,0,1.0400734542,0.7730480482,0.6014239258
Cl,0,4.1189065057,-1.1843767906,0.4983960555
H,0,3.1858165572,-0.8736215779,-0.3426286466
Cl,0,-0.9608630021,2.6704196185,0.8616720465
Cl,0,1.3226637598,-0.1458255655,-1.5802352982
H,0,-3.3798081206,-0.412586289,-1.1985649242
O,0,-2.311986198,-2.1309579968,0.5965973224
C,0,-3.7232607831,-2.3043362469,0.4696543161
H,0,-4.2678209751,-1.4463988716,0.8657635013
H,0,-4.0131453141,-2.4842338917,-0.5666286225
H,0,-3.9602762904,-3.1839744163,1.0600494298

P7(meta)

C,0,-2.0344813703,0.4264358734,-0.5368286736
C,0,-1.1491816929,-1.2561411075,1.0064130872
C,0,-2.2163301228,-0.7001599463,0.1800195142
C,0,0.1004409895,-0.7928252806,0.9317423514
C,0,-0.7481024903,1.145964232,-0.4545220194
C,0,0.4408188151,0.3037366358,-0.0097572636
H,0,-2.819414554,0.8724365103,-1.1248343921
H,0,-1.4127837366,-2.0700659088,1.6668192757
H,0,0.8981140991,-1.2213880088,1.5206065742
H,0,-0.5109031959,1.6798589391,-1.3658379895
H,0,1.2434585712,0.9340111383,0.3504595915
Cl,0,4.2924683447,-1.4332200977,0.1650338588
H,0,3.2641716268,-1.1494464349,-0.5629475399
Cl,0,-0.8841458652,2.5543348082,0.7964788708
Cl,0,1.188979729,-0.468663947,-1.5537344443
O,0,-3.3488442009,-1.4362227548,0.2425690151
C,0,-4.474459649,-0.9925644334,-0.5107508834
H,0,-4.7932291939,-0.0010760878,-0.1847598865
H,0,-4.2437619748,-0.972491864,-1.5773760293
H,0,-5.2629322805,-1.7132641697,-0.3196669076

Table S9. Cartesian coordinates of species involved in catalyzed by HCl anisole-Cl_2 reactions in simulated CCl_4 solvent at RB3LYP/6-311+G(2d,2p). The energy data for these structures are shown in Table S5.

anisole
C,0,-0.9220162655,-0.5182939385,0.
C,0,0.0009470345,0.5277879708,0.
C,0,1.3711539223,0.2462842452,0.
C,0,1.8092014447,-1.0682949972,0.
C,0,0.893600689,-2.1214162474,0.
C,0,-0.4649357021,-1.8364439096,0.
H,0,-1.9832013457,-0.324081946,0.
H,0,2.0702211816,1.0707779263,0.
H,0,2.8712128063,-1.2735954031,0.
H,0,1.2382682604,-3.1457654943,0.
H,0,-1.1871816986,-2.6417452023,0.
O,0,-0.3335391204,1.8515641599,0.
C,0,-1.7124667344,2.1997286435,0.
H,0,-2.2180445339,1.822218094,0.891314564
H,0,-1.7466424042,3.2850450046,0.
H,0,-2.2180445339,1.822218094,-0.891314564

Cl_2
Cl,0,-1.0183191956,0.,0.
Cl,0,1.0183191956,0.,0.

HCl
Cl,0,0.,0.,0.0706993744
H,0,0.,0.,-1.2106903744

anisole-Cl_2 pi-complex ortho
C,0,0.9324139163,-0.4728303647,1.1972563869
C,0,1.525378927,0.4228198703,0.2924986896
C,0,2.1035598684,-0.0629409383,-0.8808977962
C,0,2.0980407592,-1.4337851935,-1.1310976552
C,0,1.524634841,-2.3282622026,-0.2342539286
C,0,0.9436603523,-1.8395014202,0.9314862342
H,0,0.5235810265,-0.0846583922,2.1188987285
H,0,2.5577493014,0.60627768,-1.5943641034
H,0,1.5283623402,-3.388567417,-0.4414294293
H,0,0.4931559252,-2.5186666078,1.6419339497
Cl,0,-3.6841343163,0.2718640621,-0.3917279366
Cl,0,-1.7364994795,-0.1228461044,0.2091791655
H,0,2.5500283005,-1.8002702225,-2.0428654988
O,0,1.4924242605,1.7313706692,0.652340398
C,0,2.0403195941,2.6980792781,-0.241246824
H,0,1.5209177719,2.6856776934,-1.200745987
H,0,1.8917999981,3.6602147778,0.2385518037
H,0,3.1072506131,2.5302918322,-0.397722197

anisole-Cl_2 pi-complex para
C,0,-0.1268628747,1.7558471105,0.5142505454
C,0,-0.6723699205,0.8598061228,1.4324694285
C,0,-1.6880818941,-0.0154466578,1.0616421166
C,0,-2.1707932296,0.0094869401,-0.2491491298
C,0,-1.6335599504,0.9138528857,-1.1760742041
C,0,-0.6242277054,1.7764320068,-0.7953349873
H,0,0.6273420743,2.4643434606,0.8236397819
H,0,-0.3042540392,0.8399521049,2.4488860656
H,0,-2.0890515667,-0.703627516,1.7887507372
H,0,-2.023351288,0.915022764,-2.1839294989
H,0,-0.2160618842,2.4714168003,-1.5159545168
Cl,0,3.9087025321,-0.9864194534,-0.2368890055
Cl,0,2.1738416166,0.1193869451,0.0897648801
O,0,-3.1536294194,-0.8001389639,-0.7201336982
C,0,-3.7360712326,-1.75475664,0.1650464186
H,0,-4.2223292368,-1.2640672585,1.0097429901
H,0,-4.4791083237,-2.2854594791,-0.4216735981
H,0,-2.9881586575,-2.4605401721,0.5297786744

TS1
C,0,-2.9311495004,0.3739574949,-0.2820618342
C,0,-2.6119850129,-2.031232183,0.1716924113
C,0,-3.4022959238,-0.9214595236,-0.2410845289
C,0,-1.3213114088,-1.8371373589,0.5213766517
C,0,-1.6149552979,0.6237952141,0.1164194222
C,0,-0.7026405481,-0.4992327971,0.4613455292
Cl,0,0.5248752437,-0.5905126331,-0.9260480794
H,0,-3.5792244049,1.1773461562,-0.5916022036
H,0,-3.0505991142,-3.0172166286,0.187020061
H,0,-0.6783925531,-2.6522470634,0.819545152
H,0,-0.0698900249,-0.2624178726,1.3185123509
Cl,0,3.5771182181,-0.1784758185,-1.2620852694
H,0,3.1137668286,-0.0421761662,0.3824051774
Cl,0,2.6628857996,0.0657452815,1.773374576
H,0,-4.4277005618,-1.1018656842,-0.535756126
O,0,-1.0660927501,1.7930698684,0.2272590769
C,0,-1.7740132903,2.9966491307,-0.1642318204
H,0,-1.0656757526,3.7984666974,0.0005928076
H,0,-2.0436249189,2.9368657222,-1.2157024065
H,0,-2.6523180273,3.1270421638,0.4634420522

TS2
C,0,2.292094,-2.176377,0.351027
C,0,2.588865,0.24718,-0.039001
C,0,3.095182,-1.074756,0.052853
C,0,1.251206,0.458833,0.166952
C,0,0.952012,-1.99279,0.571752
C,0,0.363716,-0.659333,0.489002
Cl,0,-0.901791,-0.804621,-0.88905
H,0,2.731952,-3.161205,0.394756
H,0,0.799491,1.435763,0.102738
H,0,0.294303,-2.818886,0.798062
H,0,-0.302196,-0.417421,1.329055
Cl,0,-3.796586,0.206253,-1.139423
H,0,-3.161244,0.536895,0.391329
Cl,0,-2.547351,0.802479,1.714908
H,0,4.15236,-1.211875,-0.134108
O,0,3.507809,1.181824,-0.338737
C,0,3.067573,2.541778,-0.475953
H,0,2.63398,2.901736,0.457298
H,0,3.958397,3.112267,-0.712271
H,0,2.343985,2.631044,-1.28616

TS3
C,0,-2.1960827983,0.3226834551,-0.9212036599
C,0,-2.3869300785,-0.0564377047,1.540659839
C,0,-2.9786032739,0.0180011732,0.2375494255
C,0,-1.054187896,0.1487927192,1.6857686919
C,0,-0.8599565573,0.532877978,-0.7774633714
C,0,-0.1797867983,0.4415215855,0.5304511146
Cl,0,1.0700610228,-0.9338303072,0.3887849171
H,0,-2.6591135405,0.3772759983,-1.8977733729
H,0,-3.0329019652,-0.2897569999,2.3794332622
H,0,-0.584600233,0.0864633742,2.6620421883
H,0,-0.2411558049,0.759967249,-1.6397269628
H,0,0.4687823257,1.3095549279,0.7081839712
Cl,0,4.0870943343,-1.4960256194,0.2169027868
H,0,3.7631676175,0.2634334674,0.3290593698
Cl,0,3.4493630976,1.6517027743,0.4191902541
O,0,-4.2661251313,-0.2195034038,0.2015553347
C,0,-5.0140992913,-0.2081623437,-1.0439338848
H,0,-4.6307877034,-0.9807842291,-1.71336866
H,0,-6.0372558273,-0.4324661281,-0.7519377976
H,0,-4.9580557837,0.7800672609,-1.5044433158

TS4
C,0,-2.0982282708,-0.0597231676,0.0619274678
C,0,-1.981767833,2.1206629467,-0.9055163379
C,0,-2.6431588217,0.914463803,-0.7733505617
C,0,-0.7560271658,2.426202719,-0.252632455
C,0,-0.7731744248,0.15598377,0.7075010211
C,0,-0.1655741102,1.4938722494,0.5266853134
H,0,-2.4217922577,2.8731028177,-1.5470778763
H,0,-3.5721560934,0.7479189017,-1.2933999243
H,0,-0.2942055316,3.38838185,-0.4124406446
H,0,-0.7973940481,-0.1517489556,1.7512984924
H,0,0.8033236279,1.6429484925,0.9887724534
Cl,0,3.3510480358,0.8975858214,1.1574545608
H,0,3.4049978073,-0.4150223379,0.3087451355
Cl,0,0.4216509633,-0.9978402113,-0.0978758947
Cl,0,3.4268279797,-1.7452494193,-0.5518900811
O,0,-2.6509655053,-1.1959411211,0.3640509536
C,0,-3.9032934437,-1.6021739587,-0.2453373351
H,0,-3.7787426072,-1.6731673186,-1.3229152242
H,0,-4.1128064879,-2.5770683138,0.1763481895
H,0,-4.6875258128,-0.8960795676,0.0166227474

TS4(meta)
C,0,-1.2979260209,-2.448754009,0.1956970427
C,0,-2.8702771122,-0.8848597308,-0.6948856131
C,0,-2.4296712428,-2.2045219236,-0.5285545357
C,0,-2.1994884646,0.2347306619,-0.1468720707
C,0,-0.5508072054,-1.3386433501,0.7874463734
C,0,-1.050905799,0.0247128116,0.576177371
H,0,-0.9206731695,-3.4495452624,0.3455383392
H,0,-3.7562606843,-0.687474723,-1.2849810134
H,0,-2.9843101867,-3.0104183718,-0.9849010534
H,0,-0.3645448555,-1.5182157174,1.8504220323
H,0,-0.4369781489,0.831312337,0.9596766278
Cl,0,1.7353216843,2.2015006395,0.8733769237
H,0,2.7783060993,1.1829705462,0.2161012869
Cl,0,1.1703032818,-1.3948343158,0.0676049808
Cl,0,3.7631258945,0.1714097136,-0.4221802114
O,0,-2.7542614335,1.4230014391,-0.4236808671
C,0,-2.0929221686,2.60665874,0.0686534556
H,0,-2.0865638016,2.6093017123,1.1586255185
H,0,-1.0734797498,2.6644546337,-0.3085586297
H,0,-2.6820169167,3.4377521691,-0.3011299574

TS5
C,0,-1.722096,0.668401,0.659219
C,0,-2.441609,-1.474045,-0.391759
C,0,-2.620111,-0.071677,-0.163467
C,0,-1.389835,-2.11143,0.157355
C,0,-0.665606,0.033707,1.213411
C,0,-0.401438,-1.398866,0.984797
Cl,0,1.23522,-1.436023,0.097732
H,0,-1.861075,1.726332,0.809497
H,0,-3.158469,-1.977961,-1.022453
H,0,-1.227913,-3.165802,-0.014592
H,0,0.056979,0.582994,1.800182
H,0,-0.200472,-1.923352,1.918875
Cl,0,3.827893,-0.211117,-0.914927
H,0,2.9897,1.046389,-0.18551
Cl,0,2.216373,2.138358,0.466339
O,0,-3.64556,0.4549,-0.7684
C,0,-3.942422,1.874157,-0.664754
H,0,-3.114716,2.452171,-1.066223
H,0,-4.830592,2.013,-1.268123
H,0,-4.141517,2.134848,0.371281

TS5(meta)
C,0,-1.7840314763,-0.6115455641,0.6490517767
C,0,-2.1029924778,1.5421599895,-0.3653336059
C,0,-2.5268335034,0.2013085003,-0.162479232
C,0,-0.9594364877,2.079151433,0.2232885208
C,0,-0.5640324808,-0.1050283376,1.2851083714
C,0,-0.1825723909,1.2883918821,1.0278854778
H,0,-2.0469893264,-1.6400954065,0.8361029689
H,0,-2.7080020204,2.153296706,-1.0226843573
H,0,-0.6770938886,3.0998192069,0.015986945
H,0,-0.5782344504,-0.2925104895,2.3631081613
H,0,0.7279479908,1.6561276852,1.4751023024
Cl,0,2.77870658,1.5956778309,-0.5242167351
H,0,3.2349829196,0.1029093294,-0.5097538735
Cl,0,0.8865128426,-1.1383608172,0.7221345991
Cl,0,3.6464070859,-1.4332146945,-0.4682939156
O,0,-3.6506883448,-0.1353703012,-0.820308196
C,0,-4.1194492577,-1.4861907379,-0.705852771
H,0,-3.3746322339,-2.1843635843,-1.0885169555
H,0,-4.3614629665,-1.7232026865,0.330858979
H,0,-5.0163201133,-1.535283944,-1.3125574605

TS7(meta)
C,0,-2.0617258845,0.4786718236,-0.3713810383
C,0,-1.0768517572,-1.5830261725,0.3879650698
C,0,-2.2282505992,-0.7994300337,0.0765190833
C,0,0.2224879559,-1.1076294496,0.2795061653
C,0,-0.6997134507,0.9964108561,-0.5975246806
C,0,0.4371946004,0.1806789724,-0.1490595786
H,0,-2.8878522791,1.1256669358,-0.6175140877
H,0,-1.2543091069,-2.5912340489,0.7398635703
H,0,1.0631767132,-1.7222851228,0.5602007808
H,0,-0.5549731661,1.0087391507,-1.6962898343
H,0,1.4342693902,0.5877836566,-0.2133147125
Cl,0,3.2476695549,-0.001738893,1.5680227921
H,0,3.4416675554,-0.5168161794,-0.0279008028
Cl,0,-0.5332506671,2.7347221618,-0.1164916122
Cl,0,3.449226734,-0.9373733047,-1.438401569
O,0,-3.3967290064,-1.4279530193,0.285187026
C,0,-4.6080227135,-0.7000741241,0.0396420306
H,0,-4.6641246675,0.1775387506,0.6840421502
H,0,-4.6727049345,-0.4045087934,-1.0079965005
H,0,-5.4130772714,-1.3851771663,0.2788757482

TS8
C,0,1.8403523018,-0.7142501648,-1.3170520362
C,0,2.0829449333,0.2629878129,-0.361311669
C,0,1.0316226282,1.0611740328,0.0656265923
C,0,-0.3454202682,0.8577539931,-0.4796437641
C,0,-0.5009406916,-0.2529628494,-1.4463843701
C,0,0.5649062704,-0.9838406245,-1.8576485371
Cl,0,-0.9031742713,2.3942859939,-1.2985468897
H,0,2.6790017495,-1.307104934,-1.6582438162
H,0,-1.03384913,0.731849215,0.3751060655
H,0,-1.4915226964,-0.4101195372,-1.8421070987
H,0,0.4445067043,-1.7827824857,-2.5724344112
Cl,0,-2.3301251495,0.3405713806,2.2272896473
Cl,0,-1.6893020922,-2.2362813769,0.5698070809
H,0,-2.0690560555,-0.9554010213,1.48029705
H,0,3.0793157007,0.4014020885,0.0252560611
O,0,1.1044630469,2.0078497804,0.9551148203
C,0,2.3524766965,2.2927078976,1.6301761591
H,0,2.6750038368,1.4168478663,2.1880846696
H,0,3.1051085895,2.5971586889,0.9065625008
H,0,2.1238469746,3.1080358086,2.3049408683

TS8(meta)
C,0,0.89419199,-1.6169876836,1.689644923
C,0,1.8595879554,-0.8552770065,0.9960138584
C,0,1.5858955047,-0.1756698434,-0.1952681053
C,0,0.3064187215,-0.252868751,-0.7235752243
C,0,-0.7328434518,-1.0315572554,-0.0371591295
C,0,-0.3561318214,-1.7572719168,1.1816967912
Cl,0,-1.611009286,-2.1152717271,-1.2145036548
H,0,1.174421484,-2.1038285995,2.6118669412
H,0,0.0552055849,0.1761635695,-1.6777426978
H,0,-1.5327801652,-0.3130454396,0.2762226287
H,0,-1.1145985381,-2.3488554089,1.6717096458
Cl,0,-0.3927910128,2.5224877026,-0.1729624404
Cl,0,-3.1245245151,1.1994979855,0.7158213294
H,0,-1.9337305063,1.8933963505,0.3264550277
H,0,2.867441441,-0.7906055912,1.3840802285
O,0,2.6179525953,0.4843478577,-0.7450344548
C,0,2.4315974475,1.1231217049,-2.0209852657
H,0,3.3851785683,1.5859188815,-2.2491119076
H,0,2.1924044226,0.3815850662,-2.7843819972
H,0,1.6531835903,1.8801780087,-1.9583777664

TS9
C,0,1.8089057093,-0.817189523,-1.224841263
C,0,2.050004899,0.1837544064,-0.2229766469
C,0,1.0468313225,0.9798582696,0.1807559054
C,0,-0.325940343,0.8097291834,-0.3362887763
C,0,-0.4968566309,-0.209143183,-1.3900712938
C,0,0.5329752835,-0.9856861418,-1.8123422396
Cl,0,-0.9723946125,2.4133419387,-0.9348801938
H,0,1.2046473847,1.7440529209,0.9277794735
H,0,-0.9918397721,0.5557766823,0.514209375
H,0,-1.4757544022,-0.3046643227,-1.831414281
H,0,0.3683315477,-1.7372624346,-2.566302326
Cl,0,-2.3552237901,-0.1185916485,2.2353716328
Cl,0,-2.115324266,-2.3766920973,0.0658755311
H,0,-2.2877710098,-1.2369053232,1.2478469142
H,0,3.0502166475,0.2667036618,0.1751849317
O,0,2.8566619466,-1.5302745423,-1.5383844597
C,0,2.7726468037,-2.6000642909,-2.5151017646
H,0,2.0493740509,-3.3420747204,-2.1874850681
H,0,2.5075485555,-2.1930978016,-3.4875599267
H,0,3.7674739045,-3.0268532925,-2.5430090023

TS9(meta)
C,0,1.5046565524,-1.6932963697,-0.6579989016
C,0,2.0148383656,-0.5619041067,0.0482363092
C,0,1.2990354624,0.5966201265,0.0608243827
C,0,-0.0285092095,0.6436360729,-0.5682540513
C,0,-0.4813854059,-0.5343584224,-1.3073367644
C,0,0.28991046,-1.6834105574,-1.3116952171
Cl,0,-0.275176356,2.1647397443,-1.5438254907
H,0,1.6319210599,1.4828639665,0.5758026525
H,0,-0.7652949011,0.7772690904,0.2763842657
H,0,-1.3755107491,-0.4535612227,-1.9017249007
H,0,-0.0510240854,-2.5620697472,-1.8370035479
Cl,0,-2.2647945745,0.9817036677,1.8289459661
Cl,0,-2.6827602409,-1.6516707758,0.1784738491
H,0,-2.5397719643,-0.2798905274,1.1120089898
H,0,2.1223913527,-2.5814320006,-0.673050739
O,0,3.2121726112,-0.7708290709,0.6313076745
C,0,3.8056468031,0.3169111178,1.3497413335
H,0,4.7411156221,-0.0666036955,1.7413241448
H,0,4.0008305151,1.1578000484,0.6830909211
H,0,3.1617816821,0.6316556618,2.1716251238

TS10
C,0,-1.8824237528,1.3515660451,-0.5527119902
C,0,0.3596050004,1.7903448325,0.2659458584
C,0,-0.7930101604,2.1249853425,-0.5664114603
C,0,0.4710545867,0.591966822,0.8632999586
C,0,-1.9308439465,0.197707703,0.4013919057
C,0,-0.5747182808,-0.4413242017,0.6584559505
H,0,-2.7581986246,1.5740510379,-1.1430533338
H,0,-0.7383237693,3.0166424438,-1.1748426095
H,0,1.3555259644,0.331877725,1.4258841135
H,0,-2.2474435666,0.5780681637,1.3775482951
H,0,-0.6376888256,-1.1526686901,1.471879174
Cl,0,-0.0469608146,-1.5479441443,-0.7889791974
H,0,1.9119443325,-2.4906913133,0.0706207334
Cl,0,-3.2160405146,-1.0045858004,-0.0349348738
Cl,0,2.995336631,-2.9674785714,0.598705158
O,0,1.3138643619,2.7630042923,0.4197448246
C,0,2.4449468376,2.6532758382,-0.4601940116
H,0,2.1341005656,2.7314354511,-1.503704389
H,0,3.1016562216,3.4817008836,-0.2124411447
H,0,2.9661907541,1.7083211406,-0.3040739613

TS11
C,0,-1.0402639675,1.610807981,0.3429148328
C,0,-2.0643311118,0.966743557,1.1585816839
C,0,-2.2209853439,-0.3614344663,1.1518645311
C,0,-1.3605965221,-1.2158190941,0.2916325406
C,0,-0.0459269249,-0.5674606512,-0.1260470477
C,0,-0.0823924475,0.9000257234,-0.2724240401
Cl,0,-2.3042247368,-1.6059411479,-1.2713165483
H,0,-2.9928561566,-0.84510938,1.7323126442
H,0,-1.1845460292,-2.1944312136,0.7194537008
H,0,0.3743983705,-1.0721926362,-0.9861962352
H,0,0.7013221277,1.3864698875,-0.8335972593
Cl,0,4.1772876083,-1.3349213198,-0.8725615552
Cl,0,1.2159226489,-1.0090808843,1.2318108066
H,0,3.1655361649,-1.2221992243,-0.0731295995
H,0,-2.6967478257,1.6069395745,1.7574092653
O,0,-1.0743120067,2.9807372922,0.2972872252
C,0,-1.6231650267,3.5473975726,-0.9028600937
H,0,-1.5737713863,4.6248828367,-0.7777892266
H,0,-1.039563657,3.251088358,-1.7749804451
H,0,-2.6620349607,3.2398920908,-1.0356287218

P1
C,0,0.6662632304,2.0736941768,-0.4569449828
C,0,1.3067460012,0.9474295499,-0.9667172252
C,0,1.705094053,-0.0870557434,-0.1168129168
C,0,1.4437122269,0.0409963226,1.2586528312
C,0,0.8047781636,1.1594573,1.7629413469
C,0,0.4079257406,2.1855269415,0.9047447478
Cl,0,1.9327841928,-1.2394848121,2.3485335652
H,0,0.3714197398,2.8638933813,-1.1331156366
H,0,-1.5867909116,1.0303805831,0.2639400745
H,0,0.6191010143,1.226257098,2.8246027157
H,0,-0.077197792,3.064098113,1.3050966322
Cl,0,-2.7303529422,0.463213631,0.0463736331
Cl,0,-1.950433114,-0.7924654351,-3.3830357668
H,0,-2.2218203363,-0.3595376235,-2.1974386114
H,0,1.4916297024,0.8763846372,-2.0266042956
O,0,2.3278847603,-1.2146484043,-0.5213533137
C,0,2.5859938273,-1.391040004,-1.9150624815
H,0,1.657777299,-1.3984571317,-2.4874677272
H,0,3.2503583614,-0.612507468,-2.2925472206
H,0,3.0736635852,-2.3565843137,-1.9994240273

P2
C,0,1.6415309214,-1.7304740758,0.7607057383
C,0,2.562286082,0.3646707592,0.0107365063
C,0,2.5964715784,-0.7366096319,0.8748808185
C,0,1.5681826964,0.4566790595,-0.9659250739
C,0,0.633727016,-1.6567028322,-0.2058526038
C,0,0.6244941369,-0.5601983384,-1.0556068626
Cl,0,-0.6187477144,-0.4435342427,-2.294290143
H,0,1.6723025568,-2.5804514996,1.427958273
H,0,1.5168351404,1.2908610114,-1.6451194186
H,0,-0.0995850332,-2.4413254183,-0.3119282742
H,0,-0.6682726085,-0.42129894,1.3596912298
Cl,0,-4.8210966276,-0.7361713151,0.9151228766
H,0,-3.6384750537,-0.416039008,1.3186727999
Cl,0,-1.4261345513,0.195423262,2.2082797135
H,0,3.3745916952,-0.7887775057,1.6220112164
O,0,3.532463982,1.293956888,0.1938769505
C,0,3.5470106846,2.4461324853,-0.6485059534
H,0,2.6291506321,3.0252648766,-0.5370924233
H,0,4.3928453061,3.0402656665,-0.3182619071
H,0,3.6841791603,2.1670987991,-1.694313463

P3
C,0,2.0964225781,0.3344393049,0.4220497311
C,0,1.7427094616,1.4000376444,1.2586401849
C,0,0.6720054179,2.2179271702,0.9437188418
C,0,-0.0584852852,1.976035064,-0.2171701024
C,0,0.2782606025,0.9245501357,-1.0554843918
C,0,1.3583487017,0.0983023916,-0.7380537888
Cl,0,-1.4119983513,3.0235029495,-0.62728687
H,0,0.4047177688,3.0383632935,1.5925576006
H,0,-1.1669101558,-0.3538719697,0.4808225564
H,0,-0.2844506668,0.7494558029,-1.9604980776
H,0,1.6046134329,-0.7143646214,-1.4027332876
Cl,0,-1.9399083802,-1.205745645,1.0672112699
Cl,0,-0.6794571225,-4.025771807,-1.0224044631
H,0,-1.1572682349,-3.0850123803,-0.2788047873
H,0,2.3198519549,1.5712891629,2.1558228942
O,0,3.1621898914,-0.4056877644,0.823492708
C,0,3.5696924217,-1.5063705325,0.0118887246
H,0,2.775440781,-2.2497375473,-0.0714177892
H,0,3.8680055769,-1.1720582298,-0.9832353154
H,0,4.424188272,-1.9445957867,0.5173063517

P5'
C,0,-1.5191810712,0.7171707314,0.3303496722
C,0,-2.5291025728,-1.3526555906,-0.5164088123
C,0,-2.5877546208,0.0702771634,-0.1877877501
C,0,-1.5174916156,-2.1051649666,-0.0816089158
C,0,-0.2515915998,-0.0138776084,0.531409285
C,0,-0.4940499655,-1.4864763627,0.8195910436
Cl,0,1.0301211272,-2.4655343732,0.9051537776
H,0,-1.515297854,1.7812977031,0.4990495731
H,0,-3.3312297478,-1.7617634327,-1.1136604709
H,0,-1.4497004335,-3.159995515,-0.2995791766
H,0,0.3773154276,0.4261467269,1.2941884943
H,0,-0.8782295956,-1.5124756259,1.8434724939
Cl,0,3.840170928,1.6422191155,0.3756679902
H,0,2.7977373406,1.080174048,-0.154764487
Cl,0,0.8423506607,0.2070275756,-1.0268508853
O,0,-3.782085435,0.620974045,-0.4844077776
C,0,-3.9564223129,2.0198370254,-0.2473184424
H,0,-3.2556650378,2.6028199444,-0.8456553261
H,0,-4.9741075618,2.245992309,-0.5471603064
H,0,-3.8220748201,2.2510477755,0.8102376282

P5''
C,0,1.7913723424,0.5717806462,0.6216914026
C,0,-0.0210179175,2.0314505499,-0.0641314457
C,0,1.1598354006,1.7428014067,0.7497331736
C,0,-0.6487600053,1.045457691,-0.7446581652
C,0,1.3299807663,-0.3913152371,-0.425700659
C,0,-0.1696326438,-0.3422542835,-0.6586918549
H,0,2.6591765313,0.3230215694,1.2132102198
H,0,1.5065940055,2.4693805215,1.4678405207
H,0,-1.5720606815,1.2502621324,-1.2650571641
H,0,1.7695840553,-0.0922034725,-1.3822626902
H,0,-0.4482296545,-0.9480598561,-1.5107239731
Cl,0,-1.1100418173,-1.2467936105,0.7590214865
H,0,-2.1008590488,-2.9872368627,-0.3839674405
Cl,0,1.9717338088,-2.0640550518,-0.1534536309
Cl,0,-2.6717784259,-3.9073875678,-1.1001226376
O,0,-0.5546087166,3.2745023477,-0.1139426373
C,0,0.1776004857,4.3873825057,0.4101292198
H,0,1.1791432682,4.4383679712,-0.0169924854
H,0,-0.3857261522,5.2669104013,0.1155310635
H,0,0.2354279462,4.3481961161,1.4978916951

P5(meta)

C,0,-1.9651994944,-0.7710000595,0.4942535533
C,0,-2.0637673607,1.5656100863,-0.196841993
C,0,-2.6261337375,0.2178130721,-0.1325616764
C,0,-0.7870562499,1.8030379464,0.1215642895
C,0,-0.6962719323,-0.4192463083,1.2078429695
C,0,0.1093967254,0.6874221663,0.5439627475
H,0,-2.3465885858,-1.7729508145,0.5910854469
H,0,-2.7101281298,2.3557434281,-0.5524084986
H,0,-0.3523925228,2.785425894,0.0095288163
H,0,-0.9285718136,-0.0313073984,2.2040888129
H,0,0.9141233366,1.0130483684,1.1914266847
Cl,0,1.0175405606,0.0934594983,-0.9864008531
H,0,3.2612229417,0.4885705779,-0.4117212278
Cl,0,0.3087751648,-1.8941129003,1.5620814242
Cl,0,4.4659292607,0.8003113852,-0.0533022556
O,0,-3.8280327629,0.1236973599,-0.7524998887
C,0,-4.4580715063,-1.1563158143,-0.7714539602
H,0,-3.831059905,-1.8883977079,-1.2827595064
H,0,-4.6697245721,-1.4990562634,0.2429481817
H,0,-5.3873691279,-1.023997734,-1.3156990134

P6

C,0,2.1628259384,-0.2796695873,0.0393443648
C,0,2.1781096555,2.0370958772,0.747172917
C,0,2.8466085485,0.8701650085,0.2045441447
C,0,0.8463203198,2.1047552602,0.9029117191
C,0,0.7314378346,-0.3765075668,0.4569267603
C,0,0.005334409,0.9605997272,0.4986589512
H,0,2.7920741795,2.88581072,1.0168354412
H,0,3.893136162,0.9419774876,-0.0448434023
H,0,0.3590091408,2.9925958353,1.275587547
H,0,0.197034917,-1.1013952854,-0.1436887737
H,0,-0.9169758273,0.8756045553,1.0582274294
Cl,0,-0.6327628329,1.2712265797,-1.2701794991
H,0,-2.8236667488,0.4248291004,-1.2189794659
Cl,0,0.675909618,-1.0830148904,2.1701852353
Cl,0,-4.0291729925,-0.0422518817,-1.1420540234
O,0,2.6223984435,-1.4472112286,-0.4452139084
C,0,3.9995655599,-1.517848989,-0.821979159
H,0,4.6426482056,-1.3187549832,0.0360822782
H,0,4.1580298445,-2.5309876243,-1.1753623332
H,0,4.2161946251,-0.8079181149,-1.6211222231

P6(meta)

C,0,-1.8130747069,-2.220844459,0.2808455697
C,0,-3.1515303639,-0.1769398901,0.2703934687
C,0,-2.9842133371,-1.5984274073,0.4850102299
C,0,-2.0900546136,0.6264268737,0.0671982404
C,0,-0.6499666989,-1.4458059383,-0.2020997161
C,0,-0.7146351293,0.0511408399,0.0823165712
H,0,-1.6985524661,-3.2862452762,0.409422772
H,0,-4.1402103728,0.2573579718,0.301371249
H,0,-3.8482449214,-2.1654521321,0.8036286974
H,0,0.3006123615,-1.8456127747,0.1271738036
H,0,-0.0177034784,0.5789043866,-0.5535610756
Cl,0,-0.0046046738,0.3267366056,1.8048765819
H,0,2.2368674695,1.0384567459,1.3936012429
Cl,0,-0.53253592,-1.6102489034,-2.0737867687
Cl,0,3.4215896289,1.4514746362,1.0817187538
O,0,-2.27749937,1.9641541212,-0.0390288602
C,0,-1.2502153273,2.7893480026,-0.6023342134
H,0,-0.3636756179,2.8123608154,0.0304663013
H,0,-0.9906843151,2.460209975,-1.6090717871
H,0,-1.6774627595,3.7856030314,-0.6506271074

P7'

C,0,-1.823177872,0.8279398663,0.1408347907
C,0,-2.3653251711,-0.0636482025,1.1619121051
C,0,-1.8639043302,-1.2863550745,1.3489600562
C,0,-0.7357663749,-1.7774611933,0.5144540936
C,0,0.0663337359,-0.6747213755,-0.1602005619
C,0,-0.6757442168,0.5383281523,-0.5117136339
Cl,0,-1.4378539669,-2.8594224771,-0.8325434867
H,0,-2.2837826926,-1.9627066427,2.0788071358
H,0,-0.0843966445,-2.4530028141,1.0534167984
H,0,0.6660623686,-1.0670875278,-0.9699147165
H,0,-0.2474292468,1.1976466264,-1.248152424
Cl,0,3.4204629207,2.0099317856,-0.9419539344
Cl,0,1.4645849711,-0.2320279836,1.115588798
H,0,2.7536346906,1.2122099731,-0.1663298882
H,0,-3.202401361,0.3006063199,1.740219739
O,0,-2.5902610015,1.9192469465,-0.0480184713
C,0,-2.1678862784,2.8783905062,-1.0213444525
H,0,-2.9180285557,3.6617749463,-1.0086770219
H,0,-1.1943752791,3.2922494336,-0.7572651161
H,0,-2.1217136231,2.4254596873,-2.0122579798

P7''

C,0,-1.431014795,1.0438222315,-0.2608144227
C,0,-2.2733440555,0.1617363592,0.5438950389
C,0,-1.9166049099,-1.1064040819,0.7754773189
C,0,-0.6560182651,-1.6597213071,0.2162319388
C,0,0.3654391044,-0.6012642936,-0.1655837602
C,0,-0.1788136411,0.675104932,-0.6123819852
Cl,0,-1.0798134017,-2.6154051095,-1.3269899062
H,0,-2.5479275655,-1.7690909488,1.3489360783
H,0,-0.214944649,-2.4121571909,0.8567409735
H,0,1.1297526889,-1.0048629582,-0.8152741696
H,0,0.4465509248,1.3481520629,-1.1786124057
Cl,0,4.2703091417,1.3619103531,0.0309639316
Cl,0,1.4164244306,-0.331987679,1.4619174703
H,0,3.2531772466,0.7718367638,0.5787650222
H,0,-3.1981612305,0.5392598849,0.9513021399
O,0,-1.8662381169,2.2621367088,-0.6555052624
C,0,-3.2421530859,2.6229691354,-0.4929355286
H,0,-3.3511408009,3.5740229664,-1.003952797
H,0,-3.9016534752,1.8872090206,-0.9527852959
H,0,-3.4966151519,2.7515412362,0.5591602252

P7(meta)

C,0,-2.032656982,0.3297119905,-0.5472077987
C,0,-1.3616408625,-1.3116271803,1.1438840564
C,0,-2.3351619586,-0.738431367,0.2186665553
C,0,-0.0804369976,-0.9365588132,1.1244072275
C,0,-0.708890281,0.9642919067,-0.4216661116
C,0,0.3899133957,0.0780218367,0.1486105277
H,0,-2.7468374103,0.7868482293,-1.2116498268
H,0,-1.7194720338,-2.0655885354,1.8305745614
H,0,0.6483573301,-1.380062203,1.7865598401
H,0,-0.3804892894,1.4364758559,-1.3381812174
H,0,1.2127832395,0.6736255581,0.5214275178
Cl,0,4.7400811584,-0.5676120582,-0.5102590029
H,0,3.4905849107,-0.682848934,-0.8241374806
Cl,0,-0.8212475168,2.4566093703,0.7510977879
Cl,0,1.1727385712,-0.838365753,-1.3009082796
O,0,-3.514977588,-1.3952940328,0.2441254403
C,0,-4.5596762959,-0.9264388608,-0.6099189443
H,0,-4.8306991073,0.1002245928,-0.3606402063
H,0,-4.2575453957,-0.9851433353,-1.6564175543
H,0,-5.4044639631,-1.5837756448,-0.4335131397

Table S10. Cartesian coordinates of species involved in catalyzed by HCl anisole-Cl_2 reactions in simulated CCl_4 solvent at RPBEPBE/6-311+G(2d,2p). The energy data for these structures are shown in Table S6.

anisole
C,0,-0.9260145181,-0.5140027327,0.
C,0,0.0033519487,0.5366993917,0.
C,0,1.379846742,0.2524525439,0.
C,0,1.8176353144,-1.069010299,0.
C,0,0.8968718229,-2.1257303753,0.
C,0,-0.4681402246,-1.8378112112,0.
H,0,-1.9960071326,-0.3158417219,0.
H,0,2.0858069677,1.0831048824,0.
H,0,2.8883867503,-1.2766025421,0.
H,0,1.2431945267,-3.1589554004,0.
H,0,-1.1973509204,-2.6490396898,0.
O,0,-0.3287583307,1.8664270947,0.
C,0,-1.7195355658,2.1956702933,0.
H,0,-2.2236186835,1.8073932695,0.8988284847
H,0,-1.7664480132,3.2892002276,0.
H,0,-2.2236186835,1.8073932695,-0.8988284847

Cl_2
Cl,0,0.,0.,1.015617711
Cl,0,0.,0.,-1.015617711

HCl
Cl,0,0.,0.,0.0746377522
H,0,0.,0.,-1.2146287522

anisole-Cl_2 pi-complex ortho
C,0,-4.5304553438,2.51317938,-0.4978474336
O,0,-4.0168276899,1.2183658442,-0.1524353902
C,0,-4.9079685604,0.219883188,0.0601282761
C,0,-4.3502840292,-1.0173200971,0.471968904
C,0,-5.1858802861,-2.1330784143,0.6560744936
C,0,-6.5622156055,-2.0223007199,0.4763562258
C,0,-7.1046554236,-0.7872435259,0.0988623067
C,0,-6.2963287143,0.3335443139,-0.1080496586
H,0,-3.6533305579,3.1590904297,-0.5954892442
H,0,-5.0740566884,2.4806020421,-1.453451679
H,0,-5.1878389835,2.8989620326,0.2946137197
H,0,-3.2660761441,-1.1111134707,0.5141366391
H,0,-4.7402730634,-3.0826563816,0.9517029744
H,0,-7.2110308698,-2.8830814947,0.6313207648
H,0,-8.1822280648,-0.6897983608,-0.0383018711
H,0,-6.7481618206,1.2772021738,-0.4052974507
Cl,0,-4.250959318,-0.4028717176,2.9866563699
Cl,0,-3.9897978367,0.1739457781,5.0249040534

anisole-Cl_2 pi-complex para
C,0,-4.5092270594,2.4914528014,-0.6948624722
O,0,-3.9835146919,1.1854864484,-0.413989766
C,0,-4.8577768305,0.2058272299,-0.0725938607
C,0,-4.2783295643,-1.0497490349,0.2120949234
C,0,-5.0820382852,-2.1133080943,0.581742964
C,0,-6.4821395418,-1.9523189438,0.6856895005
C,0,-7.0504117129,-0.7010424857,0.3795829572
C,0,-6.2518337409,0.377824831,0.0095541321
H,0,-3.6396358959,3.1125299772,-0.9276437532
H,0,-5.1877844696,2.4667632596,-1.5598500156
H,0,-5.0329854697,2.9011222078,0.180747022
H,0,-3.1961937787,-1.1526247143,0.1389811491
H,0,-4.63186094,-3.0811805828,0.8012712109
H,0,-7.1213681773,-2.8139302434,0.8703645128
H,0,-8.1308033647,-0.5711045816,0.4403917087
H,0,-6.7110790946,1.3396086349,-0.2070582944
Cl,0,-6.6737361432,-1.5859387491,3.2399523537
Cl,0,-6.8526325193,-1.3967370232,5.3693369678

TS1
C,0,-2.9785595127,0.3039728811,-0.2318364246
C,0,-2.6117721589,-2.0958277772,0.2328345153
C,0,-3.4391844345,-1.0048589244,-0.1535974567
C,0,-1.298219621,-1.8758158705,0.5273355363
C,0,-1.6433389248,0.5727279692,0.0952291672
C,0,-0.706358713,-0.5291087817,0.4399588918
Cl,0,0.5073947927,-0.6410538436,-0.9649088031
H,0,-3.6539703323,1.1035449568,-0.5259356921
H,0,-3.032185385,-3.0988615887,0.2765199675
H,0,-0.6252284097,-2.6849366017,0.8083571663
H,0,-0.0295164592,-0.2618236374,1.2772879836
Cl,0,3.472589426,-0.005921643,-1.1399684147
H,0,2.9124315326,0.1444930002,0.3827474218
Cl,0,2.3265203515,0.2701364859,1.7934001538
H,0,-4.4828011196,-1.2020292573,-0.4026874565
O,0,-1.0895343166,1.7617311177,0.1443855797
C,0,-1.8556226085,2.9335528064,-0.237869721
H,0,-1.1583056363,3.7672882323,-0.1362920927
H,0,-2.1897357444,2.8391763489,-1.2781386387
H,0,-2.7076977263,3.0612381268,0.4408923169

TS2
C,0,2.2826445257,-1.9986007586,0.3806193633
C,0,2.4573692367,0.4087505948,-0.157328072
C,0,3.0353789732,-0.881064665,-0.0017557626
C,0,1.1044708572,0.5729214218,0.0758763633
C,0,0.9313433915,-1.8628436555,0.6246081554
C,0,0.2872141983,-0.5601692966,0.5015862225
Cl,0,-1.0686150435,-0.8245428269,-0.7882306055
H,0,2.7693571696,-2.9686061074,0.4689037334
H,0,0.6036500537,1.5319737977,-0.0363968018
H,0,0.3113559035,-2.7109336364,0.9114119309
H,0,-0.3826780666,-0.3033719539,1.3631718034
Cl,0,-3.9837789049,-0.3475894056,-0.77385469
H,0,-3.2957824313,-0.0176621428,0.6707411141
Cl,0,-2.5761537003,0.2729285796,1.9922544791
H,0,4.1010626168,-0.98190451,-0.2126964294
O,0,3.3209380414,1.3741800916,-0.5437393354
C,0,2.7836969204,2.696864357,-0.733904956
H,0,2.361896619,3.08372421,0.2049855537
H,0,3.6313336889,3.3139072033,-1.0422996073
H,0,2.016104951,2.6955447028,-1.520739459

TS3
C,0,-2.3387059922,0.2815124634,-1.0352393979
C,0,-2.2669864616,0.0044150263,1.4378684957
C,0,-2.9940094415,0.0331969684,0.2070513455
C,0,-0.9236976287,0.2156739167,1.4333399423
C,0,-0.9914473903,0.5017455042,-1.0419851922
C,0,-0.1892301034,0.4767936903,0.1870526093
Cl,0,1.019576765,-0.9394737666,-0.0396546906
H,0,-2.9012528247,0.2863189192,-1.9656791794
H,0,-2.8180557474,-0.2015648754,2.3542266296
H,0,-0.3480216918,0.187941028,2.3579861135
H,0,-0.4638319849,0.6923139344,-1.9763112074
H,0,0.5282217351,1.3183352274,0.2638206916
Cl,0,3.9920364307,-1.2427892411,-0.1205967047
H,0,3.5379446657,0.3535465991,0.0597354976
Cl,0,3.0618930978,1.7687617043,0.2220752697
O,0,-4.2900051214,-0.1988288763,0.3223393546
C,0,-5.1367985185,-0.2060869307,-0.8579673893
H,0,-4.8302410203,-1.0111384601,-1.5364869059
H,0,-6.143035884,-0.3941547098,-0.4780984138
H,0,-5.0956688835,0.7682708782,-1.3592488682

TS4

C,0,2.1715045062,-0.1134006942,-0.2770597407
C,0,2.2642725567,1.9491043359,0.9505148513
C,0,2.8240945716,0.7089158565,0.6390176775
C,0,1.0482290043,2.4212269768,0.3962141495
C,0,0.8511187853,0.2874442242,-0.8529582792
C,0,0.3507714372,1.6347287004,-0.4742561545
H,0,2.7949156503,2.5866376567,1.6593885677
H,0,3.7622207775,0.4064328606,1.09741044
H,0,0.6593998329,3.3932862852,0.6921693079
H,0,0.8518252579,0.1493141295,-1.9437637704
H,0,-0.6000838272,1.9485414497,-0.899788227
Cl,0,-2.4665316981,1.7044562166,1.0704694128
H,0,-2.8457538291,0.0753979656,1.1327741466
Cl,0,-0.4120069737,-0.8987924831,-0.2259308455
Cl,0,-3.1489059251,-1.3888616889,1.1701078907
O,0,2.6118728371,-1.270416077,-0.7253306331
C,0,3.8404628659,-1.822562923,-0.1845445592
H,0,3.7370342495,-1.9721711844,0.8969227664
H,0,3.9644769458,-2.7816745413,-0.6912626415
H,0,4.6830247391,-1.157523894,-0.4110222443

TS4(meta)

C,0,-1.799222267,-2.215657211,0.3670073939
C,0,-3.1796989139,-0.4137223304,-0.4337360797
C,0,-2.9895300102,-1.7816186858,-0.1646210939
C,0,-2.1930607638,0.5718579859,-0.1632122723
C,0,-0.7411374395,-1.2443005508,0.6651754595
C,0,-0.9606296394,0.1674034666,0.3263621189
H,0,-1.614338701,-3.263382862,0.598689081
H,0,-4.1116923604,-0.0760876734,-0.8909144184
H,0,-3.7879543286,-2.485716717,-0.394013718
H,0,-0.5394183847,-1.2966706197,1.7572285638
H,0,-0.1081553612,0.8467452558,0.4823900786
Cl,0,1.9314137146,1.8586726791,0.9862710502
H,0,2.8374131673,0.7528640268,0.2107619466
Cl,0,0.8680803008,-1.8003468824,-0.0437345106
Cl,0,3.6882076719,-0.2706936249,-0.5235807266
O,0,-2.5395832591,1.8332526152,-0.4755193071
C,0,-1.5358378055,2.8570279254,-0.2709538824
H,0,-1.2443181674,2.9048548975,0.7868337521
H,0,-0.6485164742,2.6590767273,-0.8863250564
H,0,-2.0126179784,3.7912355777,-0.5768413793

TS5

C,0,-1.6872238921,0.6617867759,0.6843921559
C,0,-2.407938397,-1.468180302,-0.4008993233
C,0,-2.5755077342,-0.0632870959,-0.1608719892
C,0,-1.3663842476,-2.1270224748,0.1646563727
C,0,-0.634697838,0.0115770799,1.2554657374
C,0,-0.3863851119,-1.4266850411,1.0169400971
Cl,0,1.259277328,-1.5017521105,0.1529975908
H,0,-1.8170758464,1.7290068351,0.8442276768
H,0,-3.1223979488,-1.9631903784,-1.0567359387
H,0,-1.2060625278,-3.1888219153,-0.0191281053
H,0,0.0784172096,0.5532996894,1.87514668
H,0,-0.2060695118,-1.9630474541,1.9605874168
Cl,0,3.7465611143,-0.0669205582,-0.8821032465
H,0,2.7933286939,0.9885969562,-0.304077548
Cl,0,1.7573955615,2.0713620719,0.3160768557
O,0,-3.5990685666,0.4795131978,-0.7885030075
C,0,-3.8569866288,1.9074192581,-0.6703362294
H,0,-3.0044494271,2.4738777376,-1.061824029
H,0,-4.744119518,2.0797886381,-1.2828996752
H,0,-4.0578787114,2.1676630901,0.3753685088

TS5(meta)

C,0,-1.7881285437,-0.6009336961,0.6085283215
C,0,-2.1547111437,1.6128275441,-0.2984390803
C,0,-2.541434643,0.2468740204,-0.1768114869
C,0,-1.0183631956,2.1322138807,0.3266596305
C,0,-0.5858589375,-0.1006483282,1.2802099371
C,0,-0.2075968096,1.3045549381,1.0787252665
H,0,-2.0423120882,-1.6486157615,0.7496749689
H,0,-2.7817880671,2.2555644712,-0.9181252593
H,0,-0.7577752656,3.1800151631,0.1884943905
H,0,-0.6439966968,-0.2961716114,2.3682099338
H,0,0.6858506968,1.6722472391,1.576975761
Cl,0,2.2762782339,1.4023587212,-0.7903695253
H,0,2.8998386634,-0.0132037195,-0.6281740989
Cl,0,0.8897768686,-1.1790699644,0.8475803237
Cl,0,3.4619483895,-1.5004567549,-0.41248104
O,0,-3.6555259306,-0.0845085109,-0.8683682333
C,0,-4.0748734433,-1.4596497726,-0.8137655868
H,0,-3.2881580018,-2.1213768011,-1.203583512
H,0,-4.3352334707,-1.7475394051,0.215390647
H,0,-4.961164615,-1.520509652,-1.4503693575

TS6

C,0,-2.1621850698,-0.3165068914,-0.0585847522
C,0,-0.7082220543,-2.0290139714,0.8028650063
C,0,-1.9974403963,-1.5153568354,0.6248862785
C,0,0.4615990138,-1.3942313445,0.3212729172
C,0,-0.9671640948,0.396994141,-0.628584692
C,0,0.3610567642,-0.2052348134,-0.3411249602
H,0,-0.6037293194,-2.9652781362,1.3535469093
H,0,1.4430192275,-1.8306280128,0.4949384052
H,0,-1.0894059009,0.4098869678,-1.7281377046
H,0,1.243581921,0.3106024906,-0.7172191778
Cl,0,3.2136695236,0.661609458,1.2049405436
H,0,3.4304861522,-0.0069210094,-0.1952676463
Cl,0,-0.9679519391,2.1430986776,-0.1378971351
Cl,0,3.4877678859,-0.6859722752,-1.6094399747
H,0,-2.8531392813,-2.0482306945,1.0320171036
O,0,-3.3082487766,0.2769396871,-0.3146055351
C,0,-4.5436793097,-0.3306914969,0.1475938743
H,0,-4.6714576156,-1.3177251545,-0.3134620765
H,0,-4.5369119571,-0.4056633891,1.2416508949
H,0,-5.3310327735,0.3500616025,-0.1818732785

TS7

C,0,-2.0746883617,1.3973929777,-0.5617515289
C,0,-1.6631383945,-0.922160958,-0.0177990794
C,0,-2.5691940345,0.1732180229,-0.2562357681
C,0,-0.2610530423,-0.7525314963,-0.0830263768
C,0,-0.6140163361,1.6298137492,-0.6837512122
C,0,0.264176502,0.4739354038,-0.3725633126
H,0,-2.7362656933,2.2460641104,-0.7333475133
H,0,0.3986156203,-1.5952526143,0.1185519903
H,0,-0.3845069411,1.9669456602,-1.7114461979
H,0,1.342383152,0.6095926356,-0.4232713547
Cl,0,2.6525225035,-0.423072536,1.6066095749
H,0,2.8901716627,-0.8448964894,0.0975994497
Cl,0,-0.1554674627,3.0657981645,0.3537229285
Cl,0,2.9121064777,-1.1632438858,-1.4223614228
H,0,-3.6439381797,0.0214620614,-0.1805972442
O,0,-2.0737579577,-2.1473445276,0.288101668
C,0,-3.484199668,-2.4405180846,0.4090256151
H,0,-3.9326864156,-1.8477333337,1.2164072712
H,0,-3.9996602589,-2.2577269016,-0.5426890459
H,0,-3.5289521721,-3.5033439583,0.6584715591

TS7(meta)

C,0,-2.0966154944,0.4527182053,-0.3603861648
C,0,-1.0802558294,-1.6370769574,0.3321262249
C,0,-2.2434649167,-0.8482301756,0.0639280489
C,0,0.2166048447,-1.1460241402,0.1955891658
C,0,-0.739676737,0.9824812143,-0.6000994936
C,0,0.4180210156,0.1636274497,-0.2037428948
H,0,-2.9396098982,1.1028554099,-0.5806490786
H,0,-1.2446266028,-2.6608387499,0.6724778741
H,0,1.0771064283,-1.7696924486,0.4287940798
H,0,-0.6199862686,1.0203778462,-1.7120195436
H,0,1.4175204273,0.5814002835,-0.2971845631
Cl,0,3.1305776093,0.0395929319,1.6393695745
H,0,3.3355161386,-0.4070813502,0.1578320499
Cl,0,-0.5692041585,2.7164527027,-0.0999094163
Cl,0,3.3463291536,-0.8205058674,-1.3615609223
O,0,-3.4111652012,-1.4879926712,0.2846570887
C,0,-4.6203224571,-0.736274301,0.0736087732
H,0,-4.6534803403,0.1380047842,0.7395027397
H,0,-4.7001623269,-0.4167159313,-0.975608239
H,0,-5.4365713864,-1.4209032348,0.3165806966

TS8

C,0,1.32376798,2.3719982986,-0.7130228013
C,0,1.8199257607,1.1123804103,-1.0784846085
C,0,1.355772552,-0.0157838952,-0.4160646152
C,0,0.3091987984,0.1002586432,0.6438960407
C,0,-0.2081693713,1.465633203,0.9015031171
C,0,0.3227455372,2.5577839486,0.2565198788
Cl,0,0.945119231,-0.5688397542,2.2214093031
H,0,1.7396810884,3.2490769592,-1.2112590474
H,0,-0.5302907688,-0.5974189354,0.3751554498
H,0,-0.9237468816,1.5671159344,1.713270534
H,0,-0.0375407608,3.5592095564,0.4826357273
Cl,0,-2.242499166,-1.8067110318,-0.2217359979
Cl,0,-2.7179872921,1.2769370082,-0.418587144
H,0,-2.5668446423,-0.3361053801,-0.3502368885
H,0,2.5777483908,1.0348657731,-1.8543200766
O,0,1.733314023,-1.2598386379,-0.6435420737
C,0,2.709381306,-1.5204041891,-1.6808247548
H,0,2.3217383398,-1.1909050776,-2.6527970595
H,0,3.6545606864,-1.0150174012,-1.4450024529
H,0,2.8463110092,-2.6037494506,-1.6744997032

TS8(meta)
C,0,0.7515512044,-1.8302354131,1.8341742496
C,0,1.8498941742,-1.0417492797,1.4034814416
C,0,1.7889714307,-0.2160068874,0.2753600888
C,0,0.5971143962,-0.1657534874,-0.4645551861
C,0,-0.5438065152,-1.0193231596,-0.0836614319
C,0,-0.4008910886,-1.8734577262,1.1051424227
Cl,0,-1.107814274,-1.9895349449,-1.5304897844
H,0,0.8557582715,-2.4263148448,2.7398898346
H,0,0.5491650299,0.3202049779,-1.4342491836
H,0,-1.4402469783,-0.3509303402,0.1051896635
H,0,-1.250316655,-2.4895663243,1.3942538479
Cl,0,-0.1322733604,2.3215174764,0.2779264073
Cl,0,-3.0273806764,1.0941181883,0.2521794917
H,0,-1.7420316917,1.767772185,0.2785073734
H,0,2.7912306595,-1.0781301458,1.9531287636
O,0,2.9157305697,0.4635844984,-0.0299399086
C,0,2.940809142,1.218331821,-1.2597932843
H,0,3.9316752386,1.6790154908,-1.2916283375
H,0,2.8174893593,0.5497718413,-2.1243295005
H,0,2.1656467634,1.9949820741,-1.2557579678

TS9
C,0,2.1521165418,0.1102854214,0.3792533727
C,0,1.5283197891,0.9858895874,1.3379666227
C,0,0.2749963539,1.4428798264,1.1189763104
C,0,-0.5052129126,1.0099059843,-0.0587223316
C,0,0.1808553917,0.090775646,-0.9934711165
C,0,1.4781327597,-0.3138657364,-0.7845794133
Cl,0,-1.0717280647,2.4833086225,-0.9960878113
H,0,-0.2106731763,2.1192933677,1.8213027015
H,0,-1.4694692789,0.5508370323,0.2901118401
H,0,-0.3356864317,-0.1572916372,-1.9168806976
H,0,1.9609793307,-0.9715240298,-1.5025990913
Cl,0,-3.3250144964,-0.5069795456,0.8609491384
Cl,0,-1.1687757309,-2.345347232,-0.4817901915
H,0,-2.3613756369,-1.4552875381,0.2366618608
H,0,2.1036798926,1.2684446676,2.2184503184
O,0,3.3926260734,-0.2326843783,0.6922870065
C,0,4.1320154629,-1.1271010795,-0.178814801
H,0,3.6017543623,-2.0818959976,-0.2757844402
H,0,4.2817163122,-0.6606001908,-1.160043522
H,0,5.092214458,-1.27464479,0.3200822448

TS9(meta)
C,0,1.5535470658,-1.6984334349,-0.6721492799
C,0,2.0233180382,-0.5815079797,0.0941671826
C,0,1.2885003837,0.5764124516,0.1315816822
C,0,-0.0218760521,0.6325204449,-0.5324465859
C,0,-0.4692258502,-0.5466257345,-1.2847452051
C,0,0.3418876482,-1.6843549551,-1.3361571061
Cl,0,-0.2104611931,2.1422842132,-1.5525826399
H,0,1.6044428014,1.4559245093,0.6869396499
H,0,-0.794242529,0.8271965763,0.2901317384
H,0,-1.328749305,-0.4381009493,-1.9397459536
H,0,0.0243681288,-2.5493587063,-1.9156387721
Cl,0,-2.3330450841,1.0853171586,1.6646633795
Cl,0,-2.4751663469,-1.6420918598,0.148156078
H,0,-2.4949442961,-0.2431679251,1.0071853721
H,0,2.2017558048,-2.5742753208,-0.7243375427
O,0,3.2145197622,-0.7954805382,0.7047973272
C,0,3.7571856471,0.2946392398,1.4673631035
H,0,4.7002543384,-0.0747192622,1.8786746384
H,0,3.9458984365,1.1653857065,0.8222710128
H,0,3.0767166011,0.5738113656,2.2852179206

TS10
C,0,-1.0432809132,1.9861060656,0.2021408238
C,0,-2.2691556404,-0.0103306035,-0.4594429659
C,0,-2.2010776857,1.2974493966,0.1845973567
C,0,-1.1492417595,-0.6796730885,-0.8281546085
C,0,0.1336479187,1.4233639963,-0.5346280779
C,0,0.1859234899,-0.0982112584,-0.5477334077
H,0,-0.9545309696,2.9709092045,0.6573395366
H,0,-3.1113613887,1.6994900738,0.6294431318
H,0,-1.2098343,-1.6862228051,-1.2396067132
H,0,0.0292048262,1.7020347559,-1.5998215438
H,0,0.9660465091,-0.4511541147,-1.2266140593
Cl,0,0.7826368064,-0.7829477877,1.1240059774
H,0,2.7286833189,-1.5496031645,0.4720952953
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P7''

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Supporting References

1. http://www.acdlabs.com.
2. http://www.stenutz.eu/conf/haasnoot.php.
3. Karplus M (1963) Vicinal proton coupling in nuclear magnetic resonance *J Am Chem Soc* 85(18):2870–2871.