Supporting Information

A Family of Heterotetrameric Clusters of Chloride Species and Halomethanes Holding by Two Halogen and Two Hydrogen Bonds

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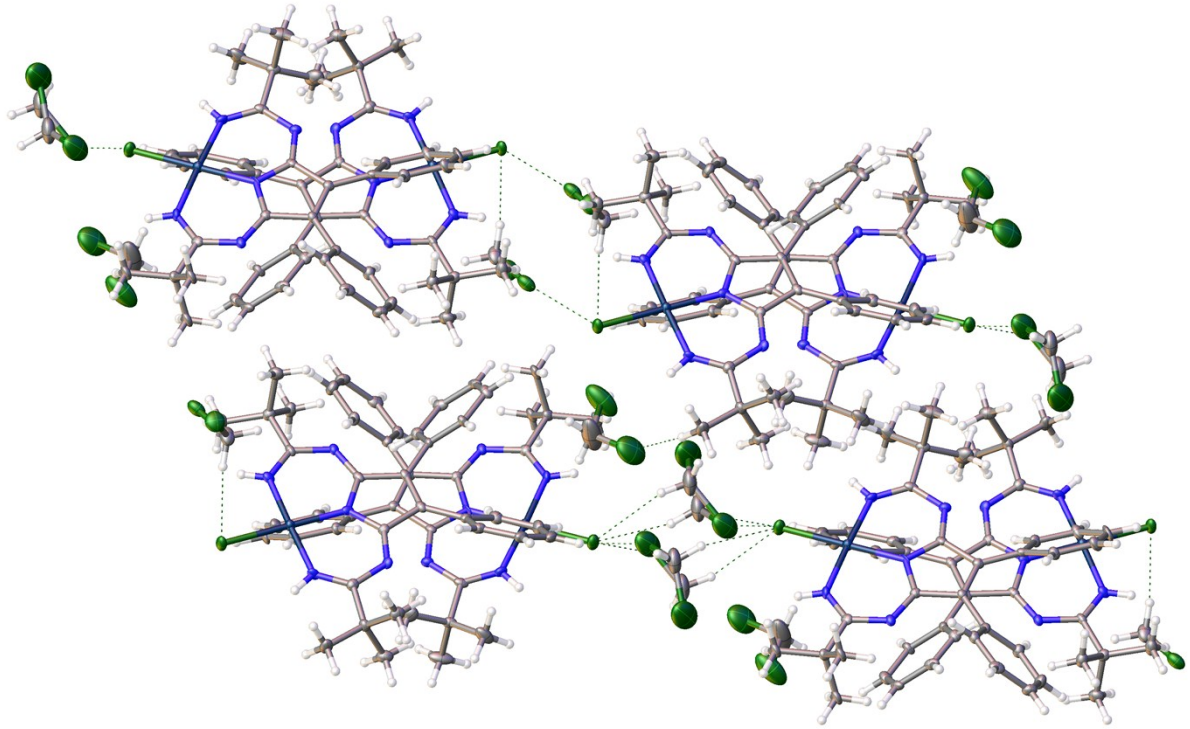
I. Packing features

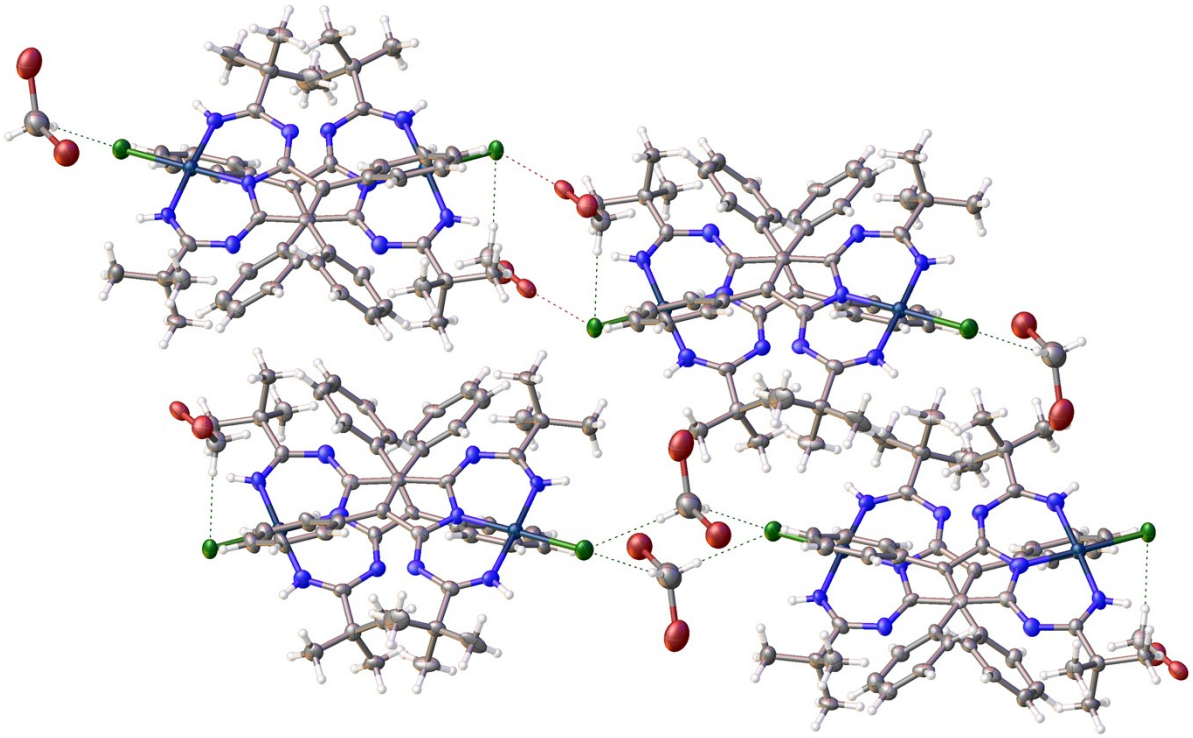
1•1¼CH_2Cl_2 and **1**•1⅖CH_2Br_2 are almost identical demonstrating close cell parameters (**Table 1S**) and the same structural features (**Figure 1S**). Difference between complex-solvent ratios can be explained in the different occupancy and positions of solvents molecules in the largest voids (solvent molecules with C2S, C3S, and C4S carbon atoms). Ratio for **1**•1⅖CH_2Br_2 was calculated by analysis of residual electron density in the cell, because unrefined positions of dibromomethane are found to be disordered, and attempts of their refinement leads to sufficient increase of R factor.

Table 1S. Crystal data and structure refinement for **1**•1¼CH_2Cl_2 and **1**•1⅖CH_2Br_2.

Structure	**1**•1¼CH_2Cl_2	**1**•1⅖CH_2Br_2	**2**•$CHCl_3$
Empirical formula	$C_{109.5}H_{131}Cl_{15}N_{20}Pt_4$	$C_{109.6}H_{131.2}Br_{11.2}Cl_4N_{20}Pt_4$	$C_{31}H_{23}Cl_4N_5Pt$
Formula weight	3039.45	3545.87	802.43
Temperature/K	100(2)	100(2)	100(2)
Crystal system	triclinic	triclinic	triclinic
Space group	P-1	P-1	P-1
a/Å	10.7179(3)	10.7918(3)	9.8061(5)
b/Å	13.6861(4)	13.7957(5)	13.1997(6)
c/Å	20.5784(7)	20.5392(5)	13.2846(6)
α/°	84.512(3)	83.691(3)	115.493(2)
β/°	87.526(2)	87.739(2)	91.131(2)
γ/°	85.480(2)	86.459(3)	107.138(2)
Volume/Å^3	2993.47(15)	3031.91(16)	1461.62(12)
Z	1	1	2
ρ_{calc}, g/cm^3	1.686	1.953	1.823
μ/mm^{-1}	5.048	13.988	5.197
F(000)	1495.0	1599.0	780.0
Crystal size/mm^3	0.22 × 0.16 × 0.08	0.26 × 0.18 × 0.12	0.41 × 0.25 × 0.12
Radiation	Mo Kα (λ = 0.71073)	Cu Kα (λ = 1.5418)	Mo Kα (λ = 0.71073)
Reflections collected	45118	61809	54027
Independent reflections	14233	12643	15564
R_{int}	0.0495	0.1384	0.0250
Goodness-of-fit on F^2	1.109	1.065	1.038
Final R indexes [I≥2σ (I)]	R_1 = 0.0465, wR_2 = 0.0945	R_1 = 0.0690, wR_2 = 0.1624	R_1 = 0.0206, wR_2 = 0.0446
Final R indexes [all data]	R_1 = 0.0648, wR_2 = 0.1022	R_1 = 0.0884, wR_2 = 0.1759	R_1 = 0.0256, wR_2 = 0.0461



1•1¼CH_2Cl_2



1•1⅖CH_2Br_2

Figure 1S. Analogous structural motifs in solvates of **1**, views along ***a*** axis. Thermal ellipsoids are shown with 50% probability.

In **2**•$CHCl_3$ (**Figure 2S**), columns consisting of π-stacked molecules of complexes were found (see next section).

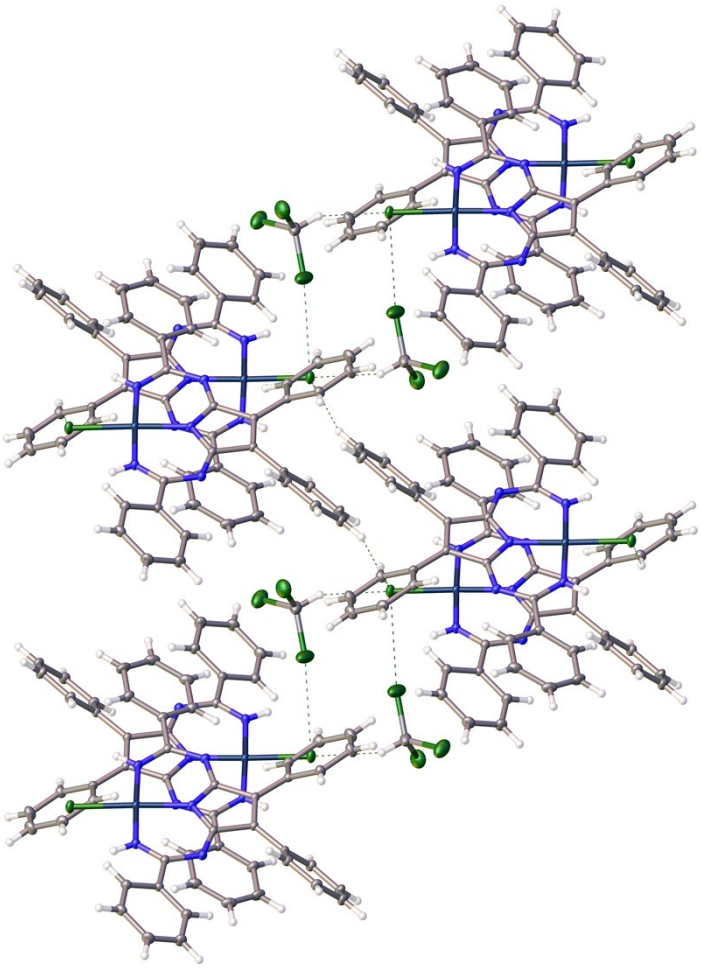


Figure 2S. **2**•$CHCl_3$, view along **a** axis. Thermal ellipsoids are shown with 50% probability.

II. Other short contacts in solvates

Other HCl_2C–H•••Cl–Pt and HBr_2C–H•••Cl–Pt hydrogen bonds. Solvates of **1** (**Figures 3S** and **4S**) contain other complex-solvent clusters, holding by only HB's. We suppose these hydrogen bonds are formed in the solvation process of the complex molecule polar parts in corresponding solutions. The characteristic parameters of the hydrogen bonds are shown in **Table 2S**.

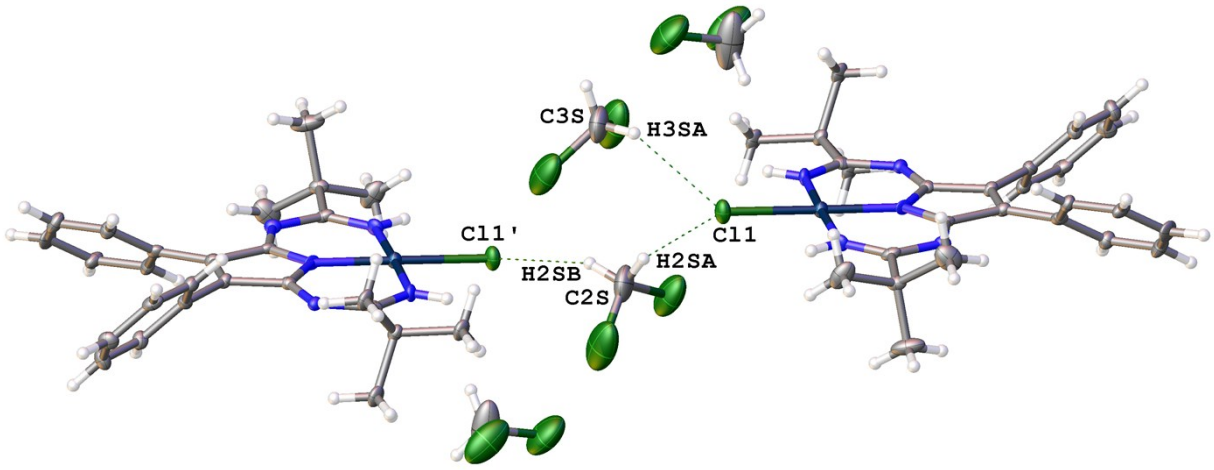


Figure 3S. The H3SA•••Cl1, H2SA•••Cl1, and H2SB•••Cl1' hydrogen bonds in one of enantiomeric heterohexamers from **1**•1¼CH_2Cl_2. The occupancies of dichloromethane molecules with the C2S and the C3S carbon atoms are 45% and 30%, respectively. Thermal ellipsoids are shown with 50% probability.

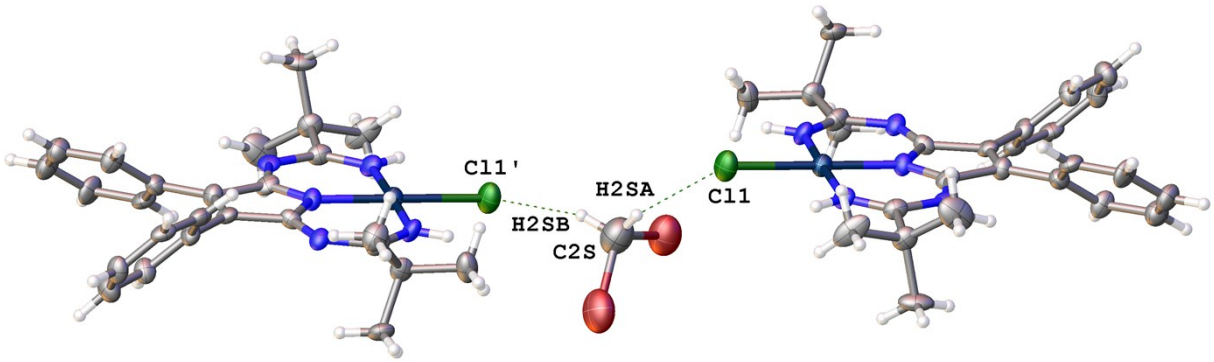


Figure 4S. The H2SA•••Cl1 and the H2SB•••Cl1' hydrogen bonds in one of enantiomeric heterotrimers from **1**•1⅖CH_2Br_2. The occupancy of dibromomethane molecule is 50%. Thermal ellipsoids are shown with 50% probability.

Table 2S. The characteristic parameters of the Pt–Cl•••H–$CClX_2$ hydrogen bonds

Solvates	C–H•••Cl	*d*(H•••Cl), Å	*d*(C•••Cl), Å	∠(Cl•••H–C), °
1•1¼CH_2Cl_2	C3S–H3SA•••Cl1	2.769	3.62(3)	146.9
	C2S–H2SA•••Cl1	2.645	3.582(16)	162.7
	C2S–H2SB•••Cl1'	2.689	3.571(18)	151.3
1•1⅓CH_2Br_2	C2S–H2SA•••Cl1	2.594	3.49(3)	152.3
	C2S–H2SB•••Cl1'	2.803	3.66(3)	148.4
	**Comparison*	*2.86*	*3.53*	*120*

*Comparison is the sums of Rowland's vdW radii and minimal hydrogen bond angle.

π-Stacking in 2•$CHCl_3$. As mentioned in section "Packing features", there are columns of π-stacked molecules of complexes in **2**•$CHCl_3$. Corresponding stacked fragment is shown on **Figure 5S**. This fragment also contains the C_{orto}–H•••Cl–Pt hydrogen bonds. The characteristic parameters of contacts are shown in **Tables 3S** and **4S**.

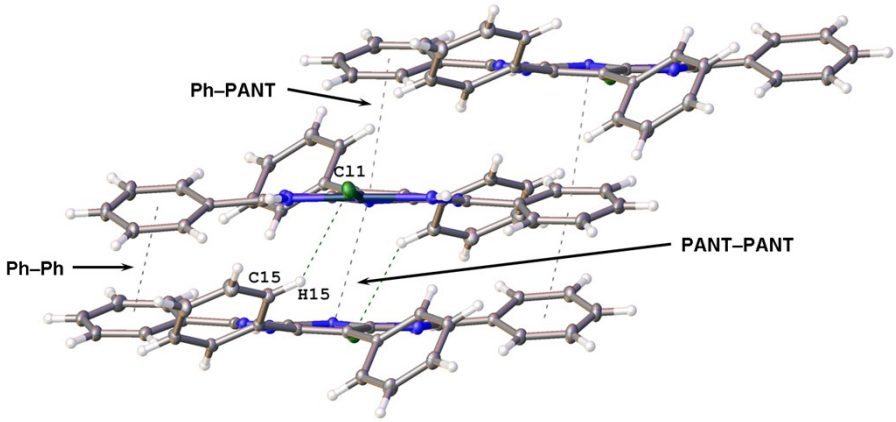


Figure 5S. π-Stacking interactions and the Pt–Cl•••H–C_{orto} hydrogen bonds in solvates of **2**•$CHCl_3$. Thermal ellipsoids are shown with 50% probability.

Table 3S. The characteristic parameters of the π-stacking interactions.

Stacking	θ,°	h_1, Å	h_2, Å	r_1, Å	r_2, Å	φ,°
Ph–Ph	7.00(5)	3.5283(14)	3.6806(13)	1.670(3)	1.300(3)	10.10(14)
Ph–PANT	18.03(4)	3.0162(18)	3.6399(9)	2.498(2)	1.4447(11)	–
PANT–PANT	0.0(3)	3.4440(8)	3.4440(8)	0.9498(11)	0.9498(11)	180.0(3)

θ is angle between ring planes;
h_i are distances between centroid of one ring to plane of another;
r_i are distances between centroid of one ring and projection of another ring centroid to first plane (shift);
φ is twist angle.

Table 4S. The characteristic parameters of the C_{orto}–H•••Cl–Pt hydrogen bonds

C–H•••Cl	*d*(H•••Cl), Å	*d*(C•••Cl), Å	∠(Cl•••H–C), °
C15–H15•••Cl1	2.796	3.5724(17)	139.6
**Comparison*	*2.86*	*3.53*	*120*

*Comparison is the sums of Rowland's vdW radii and minimal hydrogen bond angle.

III. Additional information for the theoretical consideration

Table 5S. Experimentally determined and theoretically calculated selected bond lengths and bond angles, values of the density of all electrons – ρ(**r**), Laplacian of electron density – $\nabla^2\rho(\mathbf{r})$, energy density – H_b, potential energy density – V(**r**), and Lagrangian kinetic energy – G(**r**) (Hartree) at the bond critical points (3, –1), corresponding to the non-covalent interactions in $(\mathbf{2})_2$•$(CHCl_3)_2$, $(\mathbf{1})_2$•$(CH_2Cl_2)_2$ and $(\mathbf{1})_2$•$(CH_2Br_2)_2$, as well as energies of these bonds E_{bond} (kcal/mol), defined by two methods.

Contact	Bond length / Bond Angle		ρ(**r**)	$\nabla^2\rho(\mathbf{r})$	H_b	V(r)	G(r)	E_{bond}[a]	E_{bond}[b]
	X-ray	Theory							
$(\mathbf{2})_2$•$(CHCl_3)_2$									
Cl_3C–H•••Cl–Pt, Å	2.795	2.48	0.014 0.014	0.050 0.050	0.002 0.002	–0.009 –0.009	0.011 0.011	2.8	3.0
HCl_2C–Cl•••Cl–Pt, Å	3.5012(9)	3.61	0.005 0.005	0.019 0.019	0.001 0.001	–0.003 –0.003	0.004 0.004	0.9	1.1
HCl_2C–Cl•••C(Ph), Å	3.5875(15)	3.56	0.005 0.005	0.017 0.017	0.001 0.001	–0.003 –0.003	0.003 0.003	0.9	0.8

∠(C–Cl•••Cl),°	172.16(7)	169.7							
∠(Cl•••Cl–Pt) ,°	87.902(17)	83.8							
$(\mathbf{1})_2$•$(CH_2Cl_2)_2$									
HCl_2C–H•••Cl–Pt, Å	2.809	2.63; 2.70	0.012 0.010	0.040 0.035	0.002 0.001	–0.007 –0.006	0.009 0.007	2.2 1.9	2.4 1.9
H_2ClC–Cl•••Cl–Pt, Å	3.447(2)	3.50; 3.36	0.006 0.008	0.024 0.033	0.001 0.002	–0.003 –0.005	0.005 0.006	0.9 1.6	1.4 1.6
N–H•••Cl–CH_2Cl, Å	3.017	2.80; 2.89	0.007 0.006	0.026 0.022	0.001 0.001	–0.004 –0.003	0.005 0.004	1.3 0.9	1.4 1.1
∠(C–Cl•••Cl),°	171.8(3)	168.4; 170.8							
∠(Cl•••Cl–Pt),°	108.41(7)	109.9; 108.9							
$(\mathbf{1})_2$•$(CH_2Br_2)_2$									
HBr_2C–H•••Cl–Pt, Å	2.786	3.30	Appropriate bond critical points (3, –1) were not found						
H_2BrC–Br•••Cl–Pt, Å	3.330(2)	3.17	0.014 0.014	0.050 0.050	0.002 0.002	–0.008 –0.008	0.010 0.010	2.5	2.7
N–H•••Br–CH_2Br, Å	2.983	2.69	0.011 0.011	0.036 0.036	0.001 0.001	–0.006 –0.006	0.008 0.008	1.9	2.2
∠(C–Br•••Cl),°	172.0(4)	171.0							
∠(Br•••Cl–Pt),°	107.98(8)	106.2							

[a] $E_{bond} = -V(\mathbf{r})/2$ [1]
[b] $E_{bond} = 0.429G(\mathbf{r})$ [2]

Besides bond critical points for XB's and HB's we also found two bond critical points (3, –1) between chloroform chlorine atoms and phenyl carbon atoms in $(\mathbf{2})_2$•$(CHCl_3)_2$ (**Figure 6S**, **Table 5S**). Corresponding interactions can be interpreted as the HCl_2C–Cl•••Ph weak interaction. These interactions are present in the experimental structure too, since due to geometry optimization the lengths of the appropriate short contacts changes only by 0.03 Å.

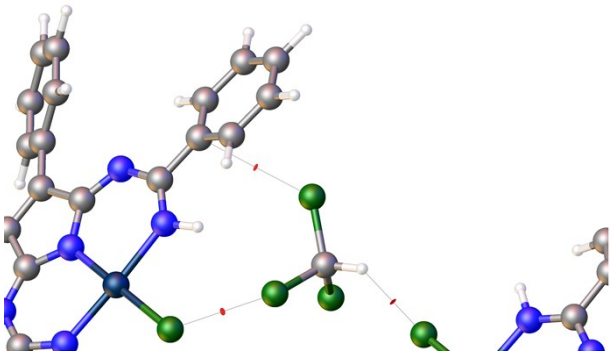


Figure 6S. The bond critical points (3, –1) around chloroform molecule in $(\mathbf{2})_2$•$(CHCl_3)_2$.

IV. Search criteria for CCDC inspection and parameters of the clusters

Searching criteria[3] for heterotetrameric clusters with covalent chlorides and chloride complexes:

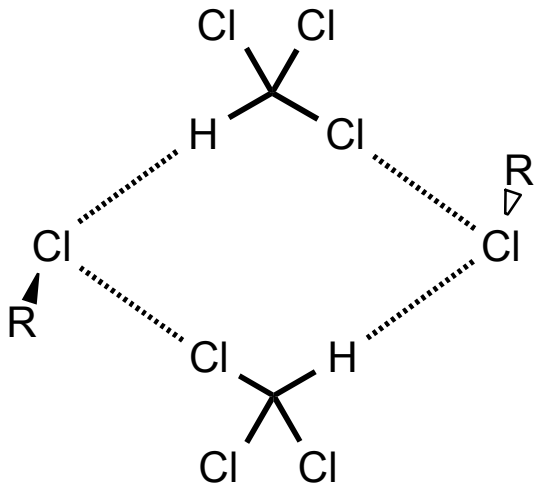
1) R < 10%;

2) No disordering;

3) XB: Cl•••Cl ≤ 3.52 Å ($\Sigma(R_w)$), ∠(CClCl) ≥ 160°, ∠(ClClR) ≤ 140°, (∠(CClCl) – ∠(ClClR)) ≥ 30°;

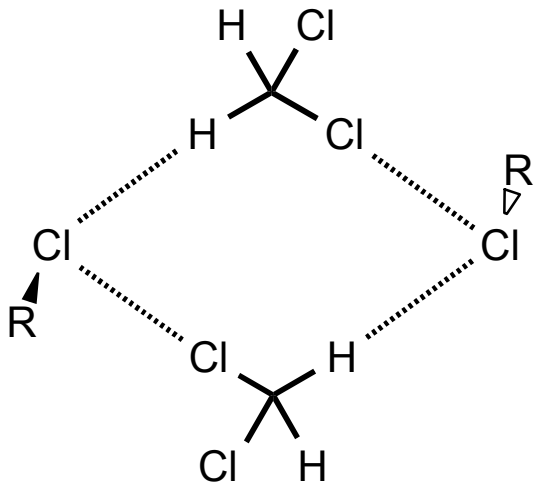
4) HB: H•••Cl ≤ 2.86 Å ($\Sigma(R_w)$), ∠(CHCl) ≥ 120°;

Table 6S. Parameters of HB's and XB's in chloride complex – chloroform clusters.



structure	R	XB			HB		
		d(Cl•••Cl), Å	∠(CClCl),°	∠(ClClR),°	d(H•••Cl), Å	d(C•••Cl), Å	∠(CHCl),°
DOKLUM	Ru(II)	3.4335(18)	167.90(17)	109.49(5)	2.684	3.527(5)	142.1
FOLJOH	Ru(II)	3.3598(6)	170.43(6)	117.321(15)	2.769	3.6119(18)	142.3
AXEXUX	Pd(II)	3.499(2)	160.18(17)	96.25(5)	2.518	3.427(5)	154.2
CIZGAU	Au(I)	3.309(3)	170.7(4)	88.14(9)	2.622	3.582(10)	160.5
DITROO	Ru(II)	3.3823(16)	166.42(15)	130.01(4)	2.613	3.568(5)	165.1
EJOHAN	Pd(II)	3.4481(6)	172.20(8)	130.72(2)	2.786	3.5706(17)	135.7
HIGLAM	Rh(III)	3.339(3)	174.4(3)	109.63(7)	2.652	3.461(8)	138.1
IPUSUI	Pd(II)	3.4282(16)	166.21(16)	112.72(4)	2.590	3.486(4)	149.2
JUGCUX	Cu(II)	3.4294(16)	163.42(14)	124.14(4)	2.698	3.577(4)	149.6
KADXUK	Pd(II)	3.419(3)	168.0(2)	127.37(6)	2.523	3.508(7)	168.3
PESMUV	Zn(II)	3.327(2)	171.89(19)	91.16(5)	2.537	3.471(4)	159.3
QATCOF	Ag(I)	3.518(2)	167.85(16)	130.52(5)	2.540	3.451(5)	154.5
	Ag(I)	3.3118(19)	176.26(16)	129.12(5)	2.522	3.435(5)	154.6
QOWGOY	Pt(II)	3.463(4)	172.3(5)	136.80(12)	2.661	3.587(12)	154.0
	Pt(II)	3.409(4)	170.2(4)	138.76(11)	2.784	3.72(1)	156.1
REPJIF	Cu(I)	3.3914(11)	167.87(10)	133.99(4)	2.825	3.778(4)	170.5
SEWMIR	Pt(II)	3.489(2)	164.8(2)	80.06(5)	2.690	3.603(6)	155.3
TULWED	Cu(II)	3.270(2)	170.5(2)	101.13(5)	2.433	3.373(7)	170.6
TUVLEC	Pt(II)	3.294(7)	169.6(8)	94.34(15)	2.649	3.59(2)	156.2
UBIFIU	Re(III)	3.460(3)	169.9(4)	101.35(7)	2.730	3.636(10)	157.4
VEKFOI	Pt(II)	3.389(2)	175.8(3)	104.44(7)	2.834	3.476(5)	122.6
VOFCAV	Re(I)	3.357(6)	166.6(7)	95.04(16)	2.622	3.492(18)	147.9
WOFLOU	Ru(I)	3.3396(12)	173.40(13)	107.89(3)	2.650	3.659(4)	172.0
WUGQOE	Zn(II)	3.5143(8)	169.36(8)	112.28(2)	2.744	3.616(2)	145.9
XESTAS	Ru(I)	3.2513(8)	160.97(8)	104.43(2)	2.796	3.713(3)	156.1
ZOVVAH	Ru(II)	3.288(4)	170.4(5)	132.62(12)	2.795	3.737(11)	154.0
Comparison		**3.52**	**180**	**90**	**2.86**	**3.52**	**120**

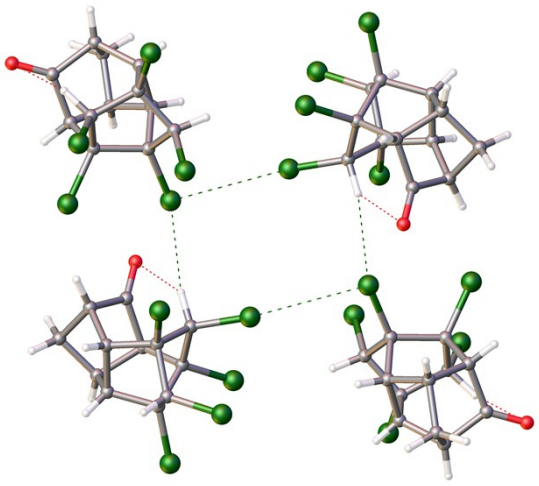
Table 7S. Parameters of HB's and XB's in chloride complex – dichloromethane clusters.



structure	R	XB			HB		
		d(Cl•••Cl), Å	∠(CClCl),°	∠(ClClR),°	d(H•••Cl), Å	d(C•••Cl), Å	∠(CHCl),°
KEVTUB	W(VI)	3.4115(12)	163.09(14)	122.24(4)	2.846	3.701(4)	145.1
VUJFAI	Hg(II)	3.4187(16)	162.60(11)	107.49(3)	2.745	3.676(4)	156.8
XIKVEU	Pd(II)	3.488(4)	165.7(3)	128.35(7)	2.761	3.657(8)	153.9
ZEQZAY	Sb(V)	3.4819(13)	160.04(11)	124.17(3)	2.785	3.628(4)	143.3
DCLMET11	C*	3.358(3)	168.71(11)	118.31(7)	2.770	3.426(6)	123.0
Comparison		**3.52**	**180**	**90**	**2.86**	**3.52**	**120**

*Parameters for cluster $(CH_2Cl_2)_4$.

Table 7S. Parameters of HB's and XB's in tetrameric cluster from KAVDUG.



XB			HB		
d(Cl•••Cl), Å	∠(CClCl),°	∠(ClClR),°	d(H•••Cl), Å	d(C•••Cl), Å	∠(CHCl),°
3.5001(19)	166.87(12)	95.35(12)	2.820	3.701(5)	142.0

Searching criteria[3] for heterotetrameric clusters with chloride anions:

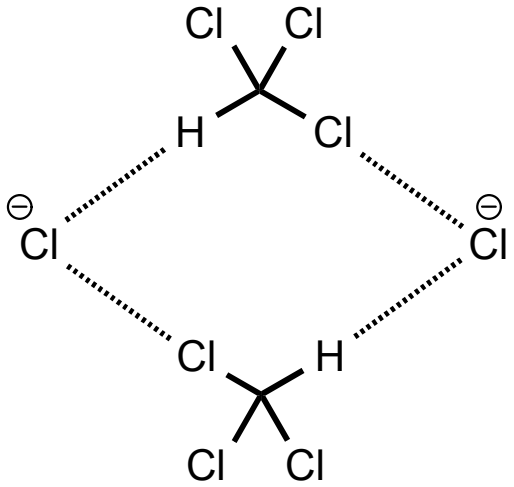
1) R < 10%;

2) No disordering;

3) XB: Cl•••Cl ≤ 3.52 Å ($\Sigma(R_w)$), ∠(CClCl) ≥ 160°;

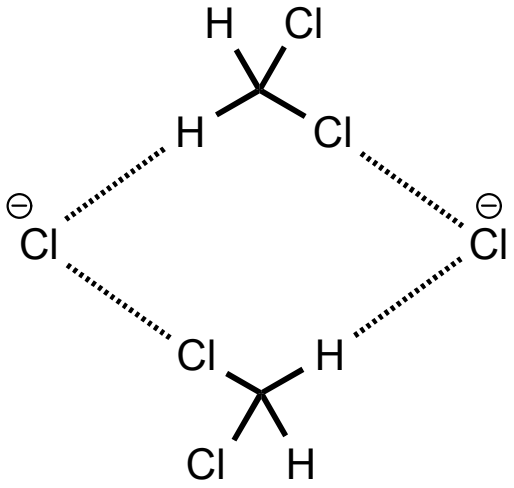
4) HB: H•••Cl ≤ 2.86 Å ($\Sigma(R_w)$), ∠(CHCl) ≥ 120°;

Table 8S. Parameters of HB's and XB's in chloride anion – chloroform clusters.



	XB		HB		
structure	d(Cl•••Cl), Å	∠(CClCl),°	d(H•••Cl), Å	d(C•••Cl), Å	∠(CHCl),°
GUJNAB	3.3827(14)	170.92(15)	2.484	3.429(5)	162.0
HIJNET	3.5077(16)	168.67(19)	2.443	3.425(6)	167.1
QAJXOP	3.4319(11)	161.30(18)	2.489	3.466(5)	165.3
RETKOR	3.2880(18)	172.2(2)	2.406	3.388(6)	167.1
TEYTEX	3.3334(19)	160.78(19)	2.392	3.365(6)	167.2
UPEROX	3.1999(17)	170.23(16)	2.541	3.509(4)	163.0
YIMVUL	3.457(2)	172.4(2)	2.434	3.396(7)	167.5
YOVYUD	3.406(3)	158.5(3)	2.356	3.444(6)	166.3
Comparison	**3.52**	**180**	**2.86**	**3.52**	**120**

Table 9S. Parameters of HB's and XB's in chloride anion – dichloromethane clusters.



	XB		HB		
structure	d(Cl•••Cl), Å	∠(CClCl),°	d(H•••Cl), Å	d(C•••Cl), Å	∠(CHCl),°
WUISEP	3.496(2)	166.23(18)	2.558	3.425(6)	146.0
ZETBOR	3.443(2)	169.7(2)	2.587	3.565(7)	169.4
Comparison	**3.52**	**180**	**2.86**	**3.52**	**120**

V. Cartesian atomic coordinates of the calculated equilibrium structures. Nuclear charges of elements are shown in the second column

Structure	Charge	X	Y	Z
$(\mathbf{2})_2$•$(CHCl_3)_2$				
	17	1.607732	-3.925325	0.951001
	17	-1.240029	-3.596534	1.560337
	17	0.086779	-1.744544	-0.281090
	6	0.275239	-2.758556	1.160878
	1	0.522679	-2.103320	2.000151
	17	-1.607732	3.925325	-0.951001
	17	1.240029	3.596534	-1.560337
	17	-0.086779	1.744544	0.281090
	6	-0.275239	2.758556	-1.160878
	1	-0.522679	2.103320	-2.000151
	78	0.404600	-1.934464	-4.364002
	17	0.330776	0.191716	-3.321903
	7	-0.984830	-1.396509	-5.692170
	1	-1.352875	-0.451097	-5.595705
	7	-1.181230	-3.403123	-6.938522
	7	0.473685	-3.710463	-5.234008
	7	2.124420	-4.778665	-3.868304
	7	1.816571	-2.556665	-3.103409
	1	2.087647	-1.899548	-2.372105
	6	-1.455091	-2.090925	-6.699630
	6	-2.377740	-1.459052	-7.673748
	6	-2.456537	-0.067855	-7.805756
	1	-1.803225	0.583354	-7.225708

	6	-3.336546	0.506348	-8.711618
	1	-3.379989	1.589395	-8.807462
	6	-4.148632	-0.300219	-9.502944
	1	-4.839452	0.150262	-10.213344
	6	-4.063897	-1.684412	-9.392633
	1	-4.688292	-2.321027	-10.016844
	6	-3.180194	-2.261350	-8.491228
	1	-3.092688	-3.341884	-8.409781
	6	-0.331937	-4.113265	-6.252789
	6	-0.063024	-5.545778	-6.522265
	6	-0.710205	-6.293617	-7.602268
	6	-2.095214	-6.227420	-7.792613
	1	-2.696448	-5.614683	-7.123305
	6	-2.700070	-6.947427	-8.815721
	1	-3.779636	-6.894859	-8.946307
	6	-1.931415	-7.734641	-9.667005
	1	-2.407004	-8.294612	-10.470351
	6	-0.552375	-7.801996	-9.489281
	1	0.056125	-8.411877	-10.154639
	6	0.053681	-7.089357	-8.464120
	1	1.133207	-7.137647	-8.327643
	6	0.903329	-5.940997	-5.648929
	6	1.479443	-7.269695	-5.435598
	6	2.839589	-7.437186	-5.143152
	1	3.481155	-6.562214	-5.067323

	6	3.364633	-8.709085	-4.950630
	1	4.425183	-8.825123	-4.733739
	6	2.543367	-9.828820	-5.033939
	1	2.958560	-10.823233	-4.878922
	6	1.188082	-9.672099	-5.311518
	1	0.536289	-10.542169	-5.365282
	6	0.661191	-8.405035	-5.512717
	1	-0.400989	-8.283051	-5.720051
	6	1.242791	-4.755434	-4.822379
	6	2.418229	-3.718254	-3.063344
	6	3.488693	-3.968372	-2.071458
	6	4.179856	-2.916742	-1.459983
	1	3.991260	-1.884012	-1.752456
	6	5.143380	-3.174766	-0.495424
	1	5.675670	-2.347348	-0.030855
	6	5.423363	-4.486216	-0.123707
	1	6.173198	-4.686944	0.639449
	6	4.751410	-5.538945	-0.737674
	1	4.972126	-6.566615	-0.454914
	6	3.796076	-5.284861	-1.712155
	1	3.265729	-6.099275	-2.200864
	78	-0.404600	1.934464	4.364002
	17	-0.330776	-0.191716	3.321903
	7	0.984830	1.396509	5.692170
	1	1.352875	0.451097	5.595705

	7	1.181230	3.403123	6.938522
	7	-0.473685	3.710463	5.234008
	7	-2.124420	4.778665	3.868304
	7	-1.816571	2.556665	3.103409
	1	-2.087647	1.899548	2.372105
	6	1.455091	2.090925	6.699630
	6	2.377740	1.459052	7.673748
	6	2.456537	0.067855	7.805756
	1	1.803225	-0.583354	7.225708
	6	3.336546	-0.506348	8.711618
	1	3.379989	-1.589395	8.807462
	6	4.148632	0.300219	9.502944
	1	4.839452	-0.150262	10.213344
	6	4.063897	1.684412	9.392633
	1	4.688292	2.321027	10.016844
	6	3.180194	2.261350	8.491228
	1	3.092688	3.341884	8.409781
	6	0.331937	4.113265	6.252789
	6	0.063024	5.545778	6.522265
	6	0.710205	6.293617	7.602268
	6	2.095214	6.227420	7.792613
	1	2.696448	5.614683	7.123305
	6	2.700070	6.947427	8.815721
	1	3.779636	6.894859	8.946307
	6	1.931415	7.734641	9.667005

	1	2.407004	8.294612	10.470351
	6	0.552375	7.801996	9.489281
	1	-0.056125	8.411877	10.154639
	6	-0.053681	7.089357	8.464120
	1	-1.133207	7.137647	8.327643
	6	-0.903329	5.940997	5.648929
	6	-1.479443	7.269695	5.435598
	6	-2.839589	7.437186	5.143152
	1	-3.481155	6.562214	5.067323
	6	-3.364633	8.709085	4.950630
	1	-4.425183	8.825123	4.733739
	6	-2.543367	9.828820	5.033939
	1	-2.958560	10.823233	4.878922
	6	-1.188082	9.672099	5.311518
	1	-0.536289	10.542169	5.365282
	6	-0.661191	8.405035	5.512717
	1	0.400989	8.283051	5.720051
	6	-1.242791	4.755434	4.822379
	6	-2.418229	3.718254	3.063344
	6	-3.488693	3.968372	2.071458
	6	-4.179856	2.916742	1.459983
	1	-3.991260	1.884012	1.752456
	6	-5.143380	3.174766	0.495424
	1	-5.675670	2.347348	0.030855
	6	-5.423363	4.486216	0.123707

	1	-6.173198	4.686944	-0.639449
	6	-4.751410	5.538945	0.737674
	1	-4.972126	6.566615	0.454914
	6	-3.796076	5.284861	1.712155
	1	-3.265729	6.099275	2.200864
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	78	-3.810453	-1.130072	-0.698635
	17	-1.841255	-2.419084	-1.007985
	7	-5.476138	-0.102381	-0.406733
	7	-2.818467	0.613317	-0.784024
	1	-1.810744	0.556116	-0.938800
	7	-7.043229	-1.905269	-0.206544
	6	-3.292063	1.822069	-0.648925
	7	-4.893870	-2.810561	-0.606880
	1	-4.375146	-3.677016	-0.744757
	6	-10.967490	-0.939479	1.175956
	1	-11.328238	-1.683651	1.883983
	6	-6.705990	-0.647606	-0.210772
	6	-9.119981	0.229086	0.135307
	6	-9.601516	-0.732158	1.031880
	1	-8.895263	-1.305459	1.628150
	6	-10.038705	0.970870	-0.617416
	1	-9.671240	1.713167	-1.324952
	6	-5.565131	1.255525	-0.349331

	6	-6.178282	-2.937219	-0.411290
	6	-11.402581	0.756673	-0.476297
	1	-12.103609	1.336694	-1.073795
	6	-11.871426	-0.198457	0.421793
	1	-12.941538	-0.364666	0.532993
	7	-4.608117	2.128278	-0.441594
	6	-7.681245	0.453533	-0.022945
	6	-7.452568	2.997769	0.033537
	6	-6.986601	1.619362	-0.117329
	6	-7.426404	5.317944	-0.657640
	1	-7.048239	6.095733	-1.318841
	6	-6.969946	4.014036	-0.800742
	1	-6.238298	3.770765	-1.567696
	6	-8.394881	3.321768	1.018106
	1	-8.766235	2.539172	1.678341
	6	-8.361749	5.628568	0.323998
	1	-8.715949	6.651711	0.437395
	6	-8.842838	4.626776	1.163083
	1	-9.569487	4.864061	1.937984
	6	-2.965304	4.063313	-1.674752
	1	-3.039336	3.642463	-2.687479
	1	-2.306538	4.940929	-1.721719
	1	-3.961773	4.394106	-1.360897
	6	-6.849122	-4.307723	-0.384670
	6	-2.382662	3.045599	-0.689167

	6	-0.960066	2.699754	-1.112388
	1	-0.470427	2.007818	-0.409870
	1	-0.349253	3.612313	-1.119904
	1	-0.927428	2.270445	-2.125102
	6	-7.957874	-4.320674	-1.442042
	1	-8.691041	-3.527708	-1.255152
	1	-8.476081	-5.289277	-1.420249
	1	-7.545585	-4.180249	-2.450910
	6	-5.874657	-5.446640	-0.667829
	1	-5.407460	-5.356410	-1.658829
	1	-6.418991	-6.399380	-0.654851
	1	-5.083269	-5.520847	0.091943
	6	-7.465751	-4.507993	1.003772
	1	-6.699080	-4.474971	1.790394
	1	-7.958345	-5.488892	1.051651
	1	-8.214539	-3.736175	1.214957
	6	-2.358737	3.653998	0.719172
	1	-3.369557	3.917926	1.053678
	1	-1.745839	4.565852	0.711112
	1	-1.914105	2.960051	1.445879
	17	-0.755854	0.291922	2.081673
	17	-1.783734	-1.799747	3.915505
	6	-1.925714	-1.037225	2.310043
	1	-2.932170	-0.624279	2.209305
	1	-1.740221	-1.791796	1.538887

	78	3.860101	1.147099	0.843645
	17	1.903540	2.420926	1.263567
	7	5.500936	0.119622	0.433188
	7	2.872247	-0.592402	0.996457
	1	1.879386	-0.528447	1.226700
	7	7.050970	1.920774	0.119873
	6	3.331775	-1.801595	0.822672
	7	4.937731	2.825829	0.684497
	1	4.433002	3.692451	0.865874
	6	10.808686	0.964269	-1.674219
	1	11.100088	1.726076	-2.395255
	6	6.710072	0.663779	0.131617
	6	9.070563	-0.220497	-0.475841
	6	9.463485	0.762161	-1.392164
	1	8.701166	1.357603	-1.890286
	6	10.055303	-0.990668	0.154603
	1	9.756194	-1.753216	0.872726
	6	5.574418	-1.236987	0.338508
	6	6.206894	2.951392	0.405948
	6	11.398813	-0.780334	-0.122755
	1	12.154169	-1.380287	0.381550
	6	11.779393	0.196921	-1.038538
	1	12.833546	0.360682	-1.255636
	7	4.624883	-2.107398	0.502853
	6	7.654335	-0.438509	-0.173600

	6	7.393544	-2.978483	-0.288883
	6	6.963389	-1.602620	-0.039537
	6	7.391233	-5.327577	0.296974
	1	7.069721	-6.129283	0.959558
	6	6.983790	-4.023795	0.548305
	1	6.345775	-3.801427	1.400817
	6	8.214312	-3.272634	-1.385321
	1	8.527160	-2.466680	-2.047866
	6	8.203238	-5.608937	-0.797055
	1	8.515373	-6.632507	-0.996934
	6	8.612358	-4.577423	-1.638052
	1	9.241153	-4.792400	-2.500169
	6	3.059871	-4.001988	1.942516
	1	3.162533	-3.544439	2.936567
	1	2.413518	-4.884371	2.043049
	1	4.048459	-4.335939	1.607332
	6	6.881696	4.319974	0.372322
	6	2.431736	-3.027105	0.941080
	6	1.023749	-2.675565	1.405401
	1	0.505508	-2.008566	0.699198
	1	0.421127	-3.591849	1.465414
	1	1.022397	-2.216279	2.405418
	6	8.010160	4.316370	1.408994
	1	8.732492	3.518426	1.202205
	1	8.537213	5.280117	1.384026

	1	7.615291	4.172554	2.424349
	6	5.917922	5.460327	0.686014
	1	5.479793	5.371903	1.690398
	1	6.463538	6.412026	0.658109
	1	5.104686	5.535546	-0.050263
	6	7.472246	4.534195	-1.024787
	1	6.691742	4.504819	-1.797824
	1	7.959381	5.517780	-1.072624
	1	8.220049	3.767658	-1.255806
	6	2.360583	-3.688738	-0.441005
	1	3.359045	-3.976342	-0.792636
	1	1.737444	-4.591569	-0.381351
	1	1.904435	-3.016566	-1.181048
	17	0.690921	-0.359235	-1.812641
	17	1.764520	1.652039	-3.710502
	6	1.895762	0.929059	-2.085448
	1	2.891760	0.492028	-1.980463
	1	1.738174	1.710431	-1.335102
$(\mathbf{1})_2 \bullet (CH_2Br_2)_2$				
	78	0.584731	1.169970	-3.147922
	17	0.385185	-1.169429	-2.808806
	7	0.613869	3.120456	-3.493309
	6	-1.239452	1.924175	-5.396701
	6	-0.030989	3.744752	-4.513043

	7	-0.686517	0.980645	-4.683147
	1	-1.020704	0.032577	-4.854592
	7	1.776240	1.490408	-1.555386
	1	1.957113	0.682248	-0.956263
	7	-0.886454	3.237807	-5.356448
	7	2.073410	3.833592	-1.742081
	6	1.166267	7.756883	-2.913691
	1	0.120431	7.769555	-3.217405
	6	1.887783	6.559213	-2.993114
	6	1.378652	4.024251	-2.817967
	6	1.244754	5.341616	-3.488151
	6	-1.369952	6.187095	-5.989498
	1	-2.102994	5.511554	-5.554889
	6	1.915929	3.650840	1.126439
	1	0.919482	3.195748	1.215875
	1	1.808054	4.651048	0.690610
	1	2.330212	3.751538	2.139272
	6	3.043049	1.433674	0.973405
	1	3.519618	1.597250	1.950153
	1	3.698145	0.756520	0.405688
	1	2.082327	0.934960	1.167733
	6	4.205707	3.462235	0.117548
	1	4.099452	4.451561	-0.341939
	1	4.886582	2.859541	-0.500111
	1	4.668541	3.587847	1.105939

	6	-1.749107	7.100564	-6.965202
	1	-2.787051	7.140039	-7.290965
	6	2.190873	2.635757	-1.090205
	6	3.102370	8.891089	-2.038259
	1	3.574205	9.798551	-1.665283
	6	2.847514	2.773742	0.277969
	6	-2.395399	1.623177	-6.344051
	6	3.226115	6.546212	-2.581455
	1	3.792894	5.619255	-2.637191
	6	3.828261	7.706836	-2.112609
	1	4.871542	7.685134	-1.802527
	6	0.379722	5.171352	-4.524648
	6	-0.041710	6.127691	-5.550489
	6	-2.067524	2.176932	-7.732692
	1	-1.854220	3.250976	-7.687672
	1	-2.919582	2.014062	-8.406797
	1	-1.192664	1.671916	-8.165151
	6	1.768636	8.912412	-2.437630
	1	1.193092	9.834085	-2.374168
	6	-0.808999	7.960412	-7.523224
	1	-1.107548	8.672633	-8.290489
	6	0.896773	6.997356	-6.120929
	1	1.935487	6.946425	-5.797827
	6	-2.693682	0.130570	-6.448319
	1	-1.832144	-0.441905	-6.820806

	1	-3.516479	-0.025568	-7.157287
	1	-3.015456	-0.296659	-5.486518
	6	-3.633544	2.334512	-5.781249
	1	-3.870832	1.997381	-4.760181
	1	-4.503320	2.117949	-6.416753
	1	-3.490626	3.421068	-5.756640
	6	0.516062	7.904079	-7.099632
	1	1.258811	8.568660	-7.537271
	35	-1.455810	1.731049	-0.124825
	35	-4.269392	1.883549	-1.702951
	6	-2.340342	1.891071	-1.842130
	1	-2.039309	2.830279	-2.309160
	1	-2.049975	1.034333	-2.452465
	78	-0.584731	-1.169970	3.147922
	17	-0.385185	1.169429	2.808806
	7	-0.613869	-3.120456	3.493309
	6	1.239452	-1.924175	5.396701
	6	0.030989	-3.744752	4.513043
	7	0.686517	-0.980645	4.683147
	1	1.020704	-0.032577	4.854592
	7	-1.776240	-1.490408	1.555386
	1	-1.957113	-0.682248	0.956263
	7	0.886454	-3.237807	5.356448
	7	-2.073410	-3.833592	1.742081
	6	-1.166267	-7.756883	2.913691

	1	-0.120431	-7.769555	3.217405
	6	-1.887783	-6.559213	2.993114
	6	-1.378652	-4.024251	2.817967
	6	-1.244754	-5.341616	3.488151
	6	1.369952	-6.187095	5.989498
	1	2.102994	-5.511554	5.554889
	6	-1.915929	-3.650840	-1.126439
	1	-0.919482	-3.195748	-1.215875
	1	-1.808054	-4.651048	-0.690610
	1	-2.330212	-3.751538	-2.139272
	6	-3.043049	-1.433674	-0.973405
	1	-3.519618	-1.597250	-1.950153
	1	-3.698145	-0.756520	-0.405688
	1	-2.082327	-0.934960	-1.167733
	6	-4.205707	-3.462235	-0.117548
	1	-4.099452	-4.451561	0.341939
	1	-4.886582	-2.859541	0.500111
	1	-4.668541	-3.587847	-1.105939
	6	1.749107	-7.100564	6.965202
	1	2.787051	-7.140039	7.290965
	6	-2.190873	-2.635757	1.090205
	6	-3.102370	-8.891089	2.038259
	1	-3.574205	-9.798551	1.665283
	6	-2.847514	-2.773742	-0.277969
	6	2.395399	-1.623177	6.344051

	6	-3.226115	-6.546212	2.581455
	1	-3.792894	-5.619255	2.637191
	6	-3.828261	-7.706836	2.112609
	1	-4.871542	-7.685134	1.802527
	6	-0.379722	-5.171352	4.524648
	6	0.041710	-6.127691	5.550489
	6	2.067524	-2.176932	7.732692
	1	1.854220	-3.250976	7.687672
	1	2.919582	-2.014062	8.406797
	1	1.192664	-1.671916	8.165151
	6	-1.768636	-8.912412	2.437630
	1	-1.193092	-9.834085	2.374168
	6	0.808999	-7.960412	7.523224
	1	1.107548	-8.672633	8.290489
	6	-0.896773	-6.997356	6.120929
	1	-1.935487	-6.946425	5.797827
	6	2.693682	-0.130570	6.448319
	1	1.832144	0.441905	6.820806
	1	3.516479	0.025568	7.157287
	1	3.015456	0.296659	5.486518
	6	3.633544	-2.334512	5.781249
	1	3.870832	-1.997381	4.760181
	1	4.503320	-2.117949	6.416753
	1	3.490626	-3.421068	5.756640
	6	-0.516062	-7.904079	7.099632

	1	-1.258811	-8.568660	7.537271
	35	1.455810	-1.731049	0.124825
	35	4.269392	-1.883549	1.702951
	6	2.340342	-1.891071	1.842130
	1	2.039309	-2.830279	2.309160
	1	2.049975	-1.034333	2.452465
$(Cl^{-})_2 \bullet (CHCl_3)_2$				
	6	-2.045830	-0.556233	0.085991
	17	-2.007311	-0.204497	1.834198
	17	-3.593994	-1.358871	-0.329351
	17	-0.677238	-1.568308	-0.378449
	1	-2.036300	0.408112	-0.437915
	6	2.044863	0.556511	0.086191
	17	2.004317	0.201649	1.833628
	17	3.594308	1.358289	-0.326287
	17	0.677778	1.571018	-0.377775
	1	2.034867	-0.406794	-0.439483
	17	2.651610	-2.530200	-1.132862
	17	-2.649046	2.530745	-1.132262
$(Cl^{-})_2 \bullet (CHCl_3) + CHCl_3$ (starting)				
	6	-4.493675	-1.291922	-0.076959
	17	-5.398935	-0.994598	-1.556735

	17	-5.600134	-1.786297	1.199353
	17	-3.658793	0.180008	0.406808
	1	-3.740714	-2.104380	-0.255374
	17	-2.472888	2.270806	1.093973
	17	-2.198020	-3.338486	0.056198
	6	4.695535	0.582746	-0.287055
	17	5.793216	1.253984	-1.487958
	17	5.533404	0.427210	1.252886
	17	4.142116	-1.001573	-0.817424
	1	3.811806	1.263281	-0.165543
$(Cl^{-})_2$•$(CHCl_3)$+$CHCl_3$ (final)				
	6	-7.518599	-4.508510	-0.488122
	17	-8.510922	-3.803403	-1.786330
	17	-8.378758	-4.397223	1.067498
	17	-5.953275	-3.673357	-0.384576
	1	-7.346629	-5.578971	-0.718459
	17	5.998194	6.762263	1.001266
	17	-7.091241	-7.614226	-1.186120
	6	6.998247	3.766586	0.393705
	17	7.868807	3.775924	-1.159288
	17	8.101152	3.295602	1.709325
	17	5.620339	2.645863	0.316205
	1	6.625605	4.790231	0.597065

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