Identification and H(D)-bond Energies of C–H(D)···Cl Interactions in Chloride–Haloalkane Clusters: Combined X-ray Crystallographic, Spectroscopic, and Theoretical Study

Tatiyana V. Serebryanskaya,[a] Alexander S. Novikov,[a] Pavel V. Gushchin,[a] Matti Haukka,[b] Ruslan E. Asfin,[c] Peter M. Tolstoy,[a] Vadim Yu. Kukushkin [a,d] *

[a.] *Institute of Chemistry, Saint Petersburg State University, 7/9 Universitetskaya Nab., 199034 Saint Petersburg, Russian Federation. E-mail: v.kukushkin@spbu.ru.*
[b.] *Department of Chemistry, University of Jyväskylä, P.O. Box 35, FI-40014 Jyväskylä, Finland.*
[c.] *Department of Physics Saint Petersburg State University, 7/9 Universitetskaya Nab., 199034 Saint Petersburg, Russian Federation.*
[d.] *Institute of Macromolecular Compounds of Russian Academy of Sciences, Bolshoii Pr. 31, 199004 Saint Petersburg, Russian Federation.*

Table S1. Crystallographic and refinement data.

Compound	[**1**][$Cl_2(CHBr_3)_4$]	[**1**][$Cl_2(CH_2Cl_2)_2$]	[**1**][$Cl_2(C_2H_4Cl_2)_2$]	[**1**][$Cl_2(CDCl_3)_4$]
Empirical formula	$C_{42}H_{50}Br_{12}Cl_2N_{10}Pt$	$C_{40}H_{50}Cl_6N_{10}Pt$	$C_{42}H_{54}Cl_6N_{10}Pt$	$C_{42}H_{46}Cl_{14}D_4N_{10}Pt$
Formula weight	1919.83	1078.69	1106.74	1386.31
T (K)	100(2)	100(2)	100(2)	100(2)
λ(Å)	0.71073	0.71073	0.71073	0.71073
Cryst syst	Orthorhombic	Triclinic	Monoclinic	Orthorhombic
Space group	Pbca	$P\bar{1}$	$P2_1/c$	Pbca
a (Å)	14.2649(5)	12.9443(5)	9.3446(5)	13.1946(2)
b (Å)	18.1921(5)	13.0808(5)	9.4052(6)	17.8886(2)
c (Å)	23.1012(7)	15.1903(6)	26.2178(17)	23.6588(3)
α (deg)	90	109.653(2)	90	90
β(deg)	90	113.249(2)	92.274(3)	90
γ(deg)	90	92.700(2)	90	90
V (Å^3)	5995.0(3)	2176.92(15)	2302.4(2)	5584.25(13)
Z	4	2	2	4
ρ_{calc} (Mg/m^3)	2.127	1.646	1.596	1.649
μ(Mo Kα) (mm^{-1})	10.467	3.634	3.438	3.223
No. reflns.	35250	21401	14065	87106
Unique reflns.	7682	7299	4156	8161
GOOF (F^2)	1.115	1.076	1.160	1.024
R_{int}	0.0514	0.0841	0.0858	0.0402
R1[a] ($I \geq 2\sigma$)	0.0587	0.0601	0.0735	0.0288
wR2[b] ($I \geq 2\sigma$)	0.1140	0.1129	0.1266	0.0545

[a] $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR2 = [\Sigma[w(F_o^2 - F_c^2)^2]/\ \Sigma[w(F_o^2)^2]]^{1/2}$.

Table S2. Selected bond lengths [Å] and angles [°] for solvates.

Solvate	[**1**][$Cl_2(CDCl_3)_4$]	[**1**][$Cl_2(CHBr_3)_4$]	[**1**][$Cl_2(C_2H_4Cl_2)_2$]	[**1**][$Cl_2(CH_2Cl_2)_2$]
Pt(1)–N(2)	2.001(2)	2.009(6)	2.000(9)	2.019(6)
Pt(1)–N(2B)				1.999(6)
Pt(1)–N(1)	2.015(2)	2.006(6)	2.037(9)	1.997(7)
Pt(1)–N(1B)				2.014(6)
N(1)–C(7)	1.303(3)	1.301(9)	1.263(14)	1.319(10)
N(2)–C(14)	1.295(3)	1.298(9)	1.282(13)	1.294(10)
N(3)–C(7)	1.336(3)	1.329(9)	1.328(14)	1.324(10)
N(4)–C(14)	1.404(3)	1.399(9)	1.428(12)	1.411(10)
N(4)–C(7)	1.413(3)	1.416(9)	1.436(13)	1.410(10)
N(5)–C(14)	1.346(3)	1.348(9)	1.353(12)	1.329(9)
N(2)–Pt(1)–N(1)	86.48(8)	85.8(2)	83.9(4)	84.0(3)
C(7)–N(1)–Pt(1)	122.96(17)	124.0(5)	124.3(8)	123.8(6)
C(14)–N(2)–Pt(1)	122.88(17)	123.0(5)	122.7(7)	122.4(6)
C(14)–N(4)–C(7)	121.7(2)	121.7(6)	119.4(9)	119.3(7)
N(1)–C(7)–N(4)	121.2(2)	120.9(6)	119.3(11)	118.4(8)
N(2)–C(14)–N(4)	120.3(2)	120.8(6)	119.7(9)	119.0(7)

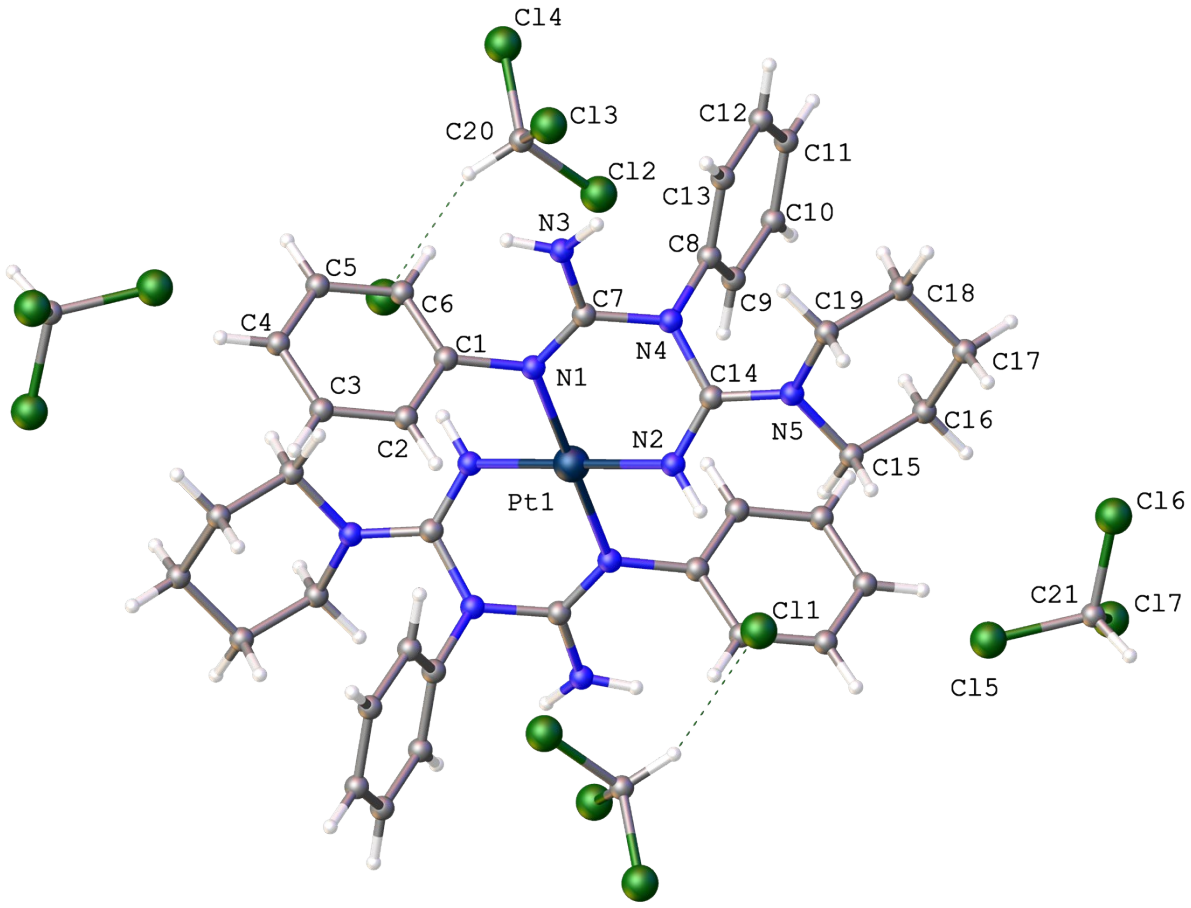

Figure S1. Molecular structure of [**1**][$Cl_2(CDCl_3)_4$] with an atom numbering scheme.

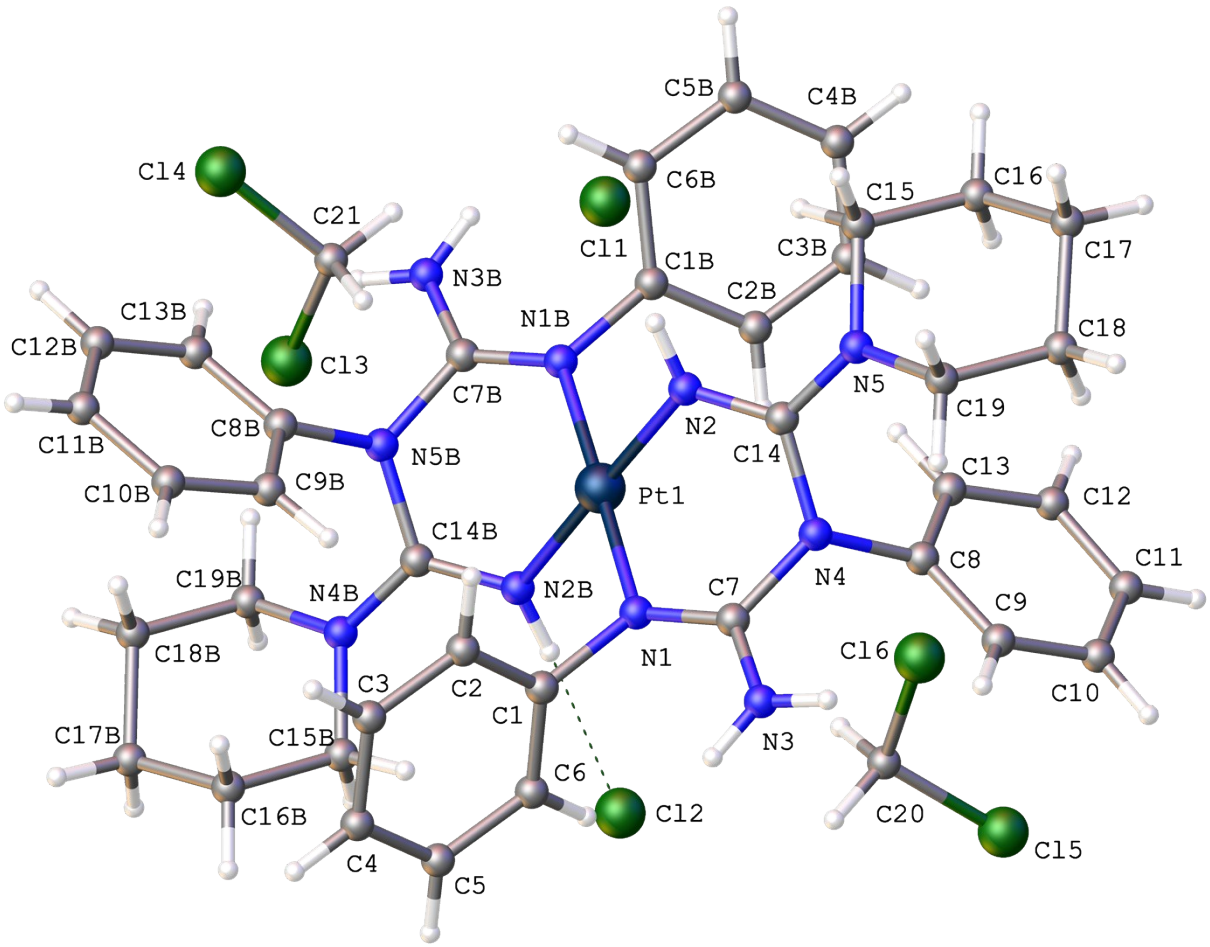

Figure S2. Molecular structure of [**1**][$Cl_2(CH_2Cl_2)_2$] with an atom numbering scheme.

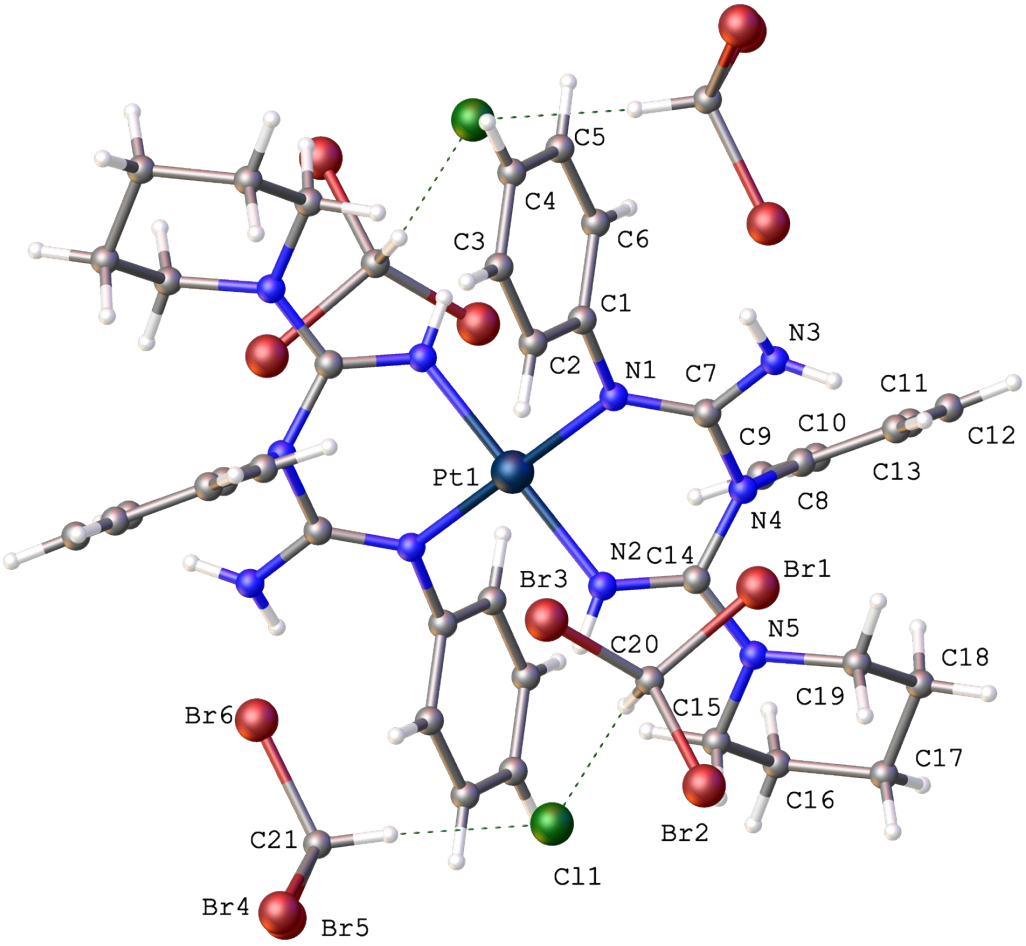

Figure S3. Molecular structure of [**1**][$Cl_2(CHBr_3)_4$] with an atom numbering scheme.

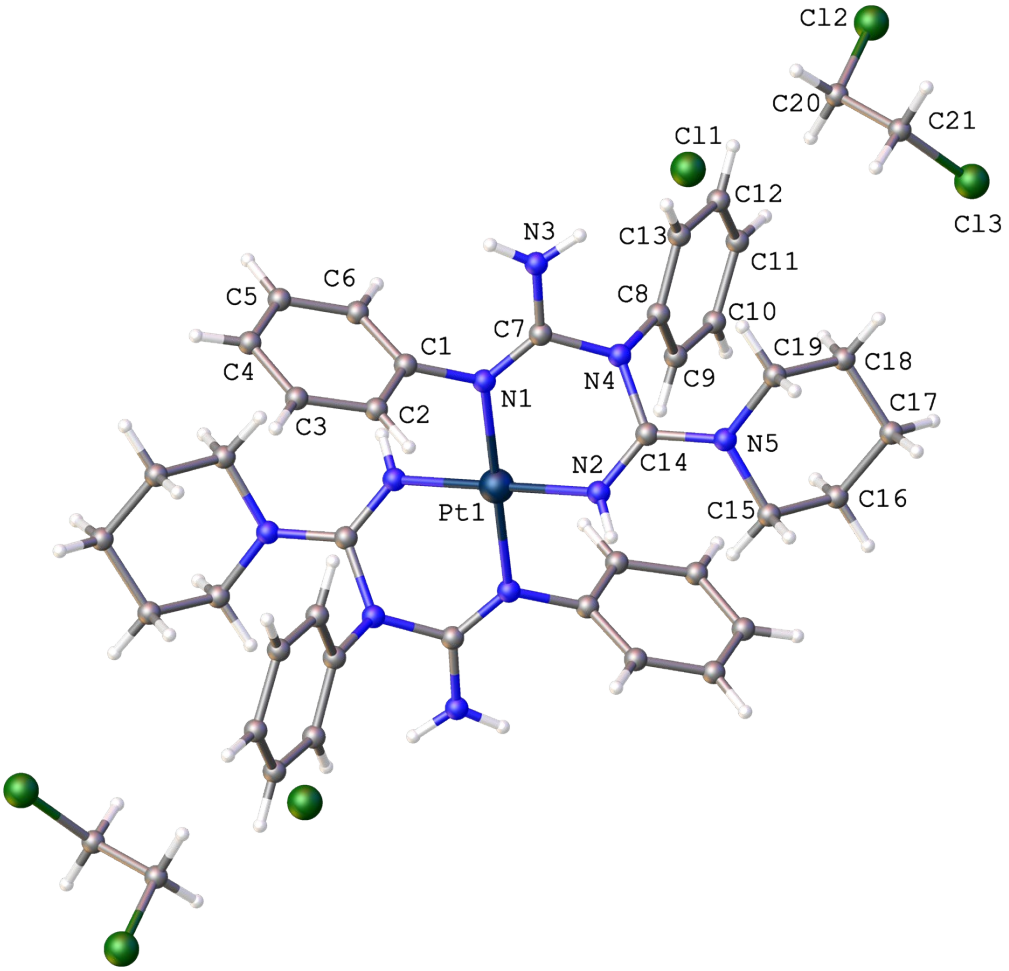

Figure S4. Molecular structure of [**1**][$Cl_2(C_2H_4Cl_2)_2$]with an atom numbering scheme.

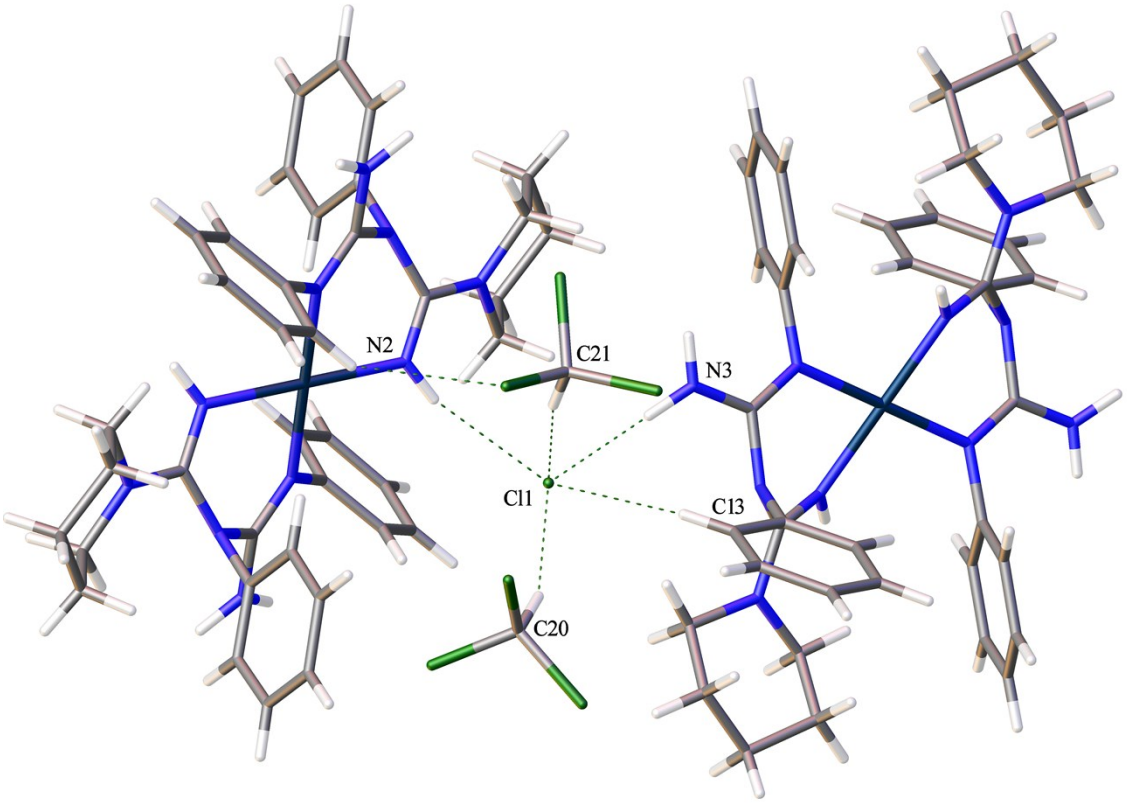

Figure S5. Hydrogen bondings in the structure of [**1**][$Cl_2(CDCl_3)_4$]showing a pyramidal environment of Cl^- anion and the $[Cl(CDCl_3)_2]^-$ cluster.

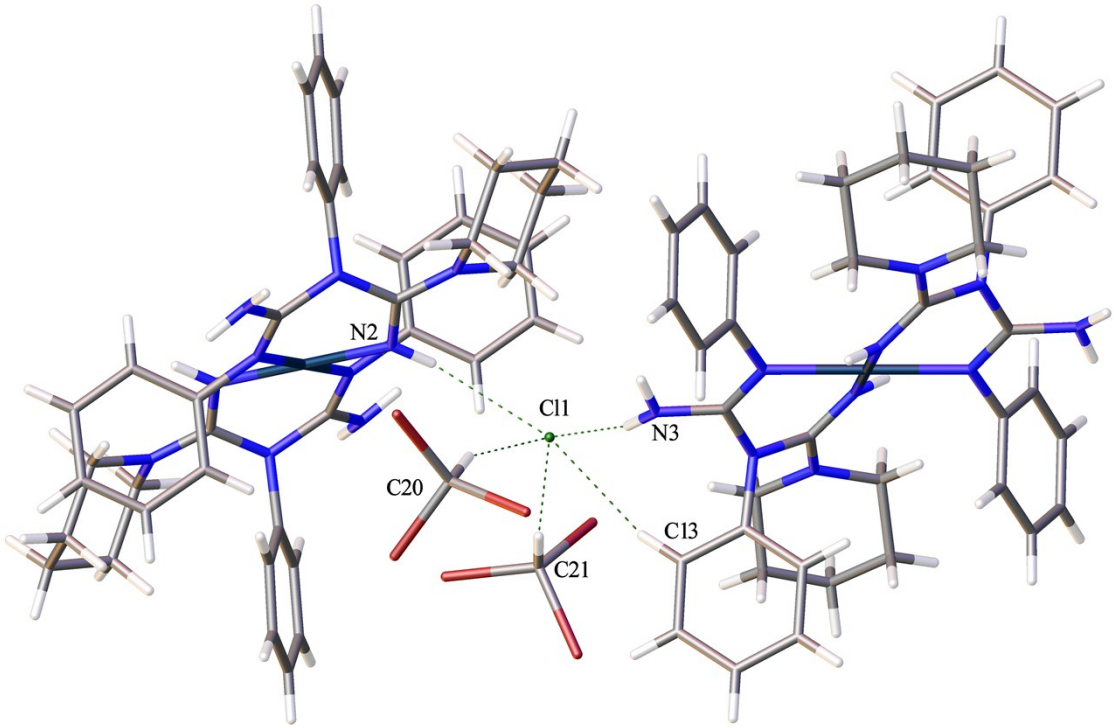

Figure S6. Intermolecular hydrogen bondings in the structure of [**1**][$Cl_2(CHBr_3)_4$]showing a pyramidal environment of Cl^- anion and the $[Cl(CHBr_3)_2]^-$ cluster.

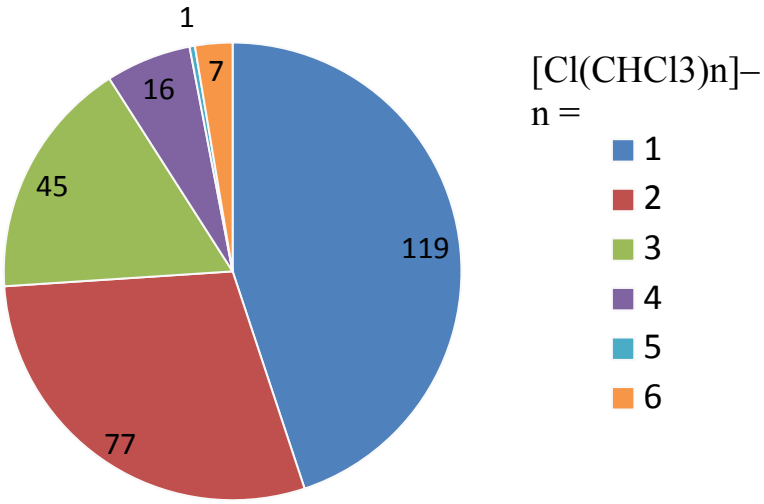

Figure S7. The distribution of the chloride-chloroform clusters $[Cl(CHCl_3)_n]^-$ depending on the number of H-bonded chloroform molecules *n* (according to the CCDC database).

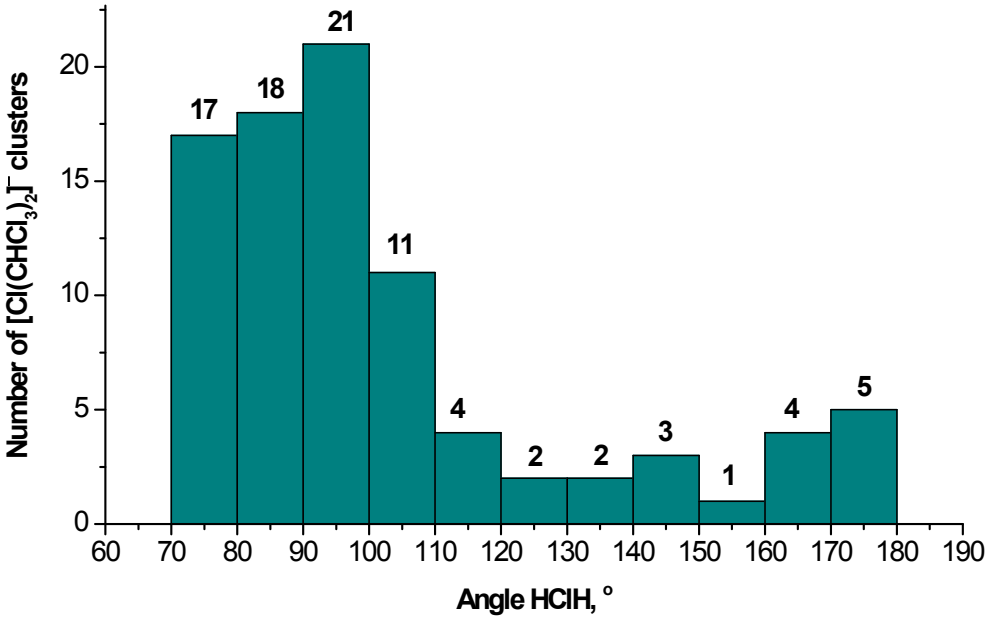

Figure S8. The distribution of dimericchloride-chloroform clusters $[Cl(CHCl_3)_2]^-$ depending on the value of HClH angle (according to the CCDC database).

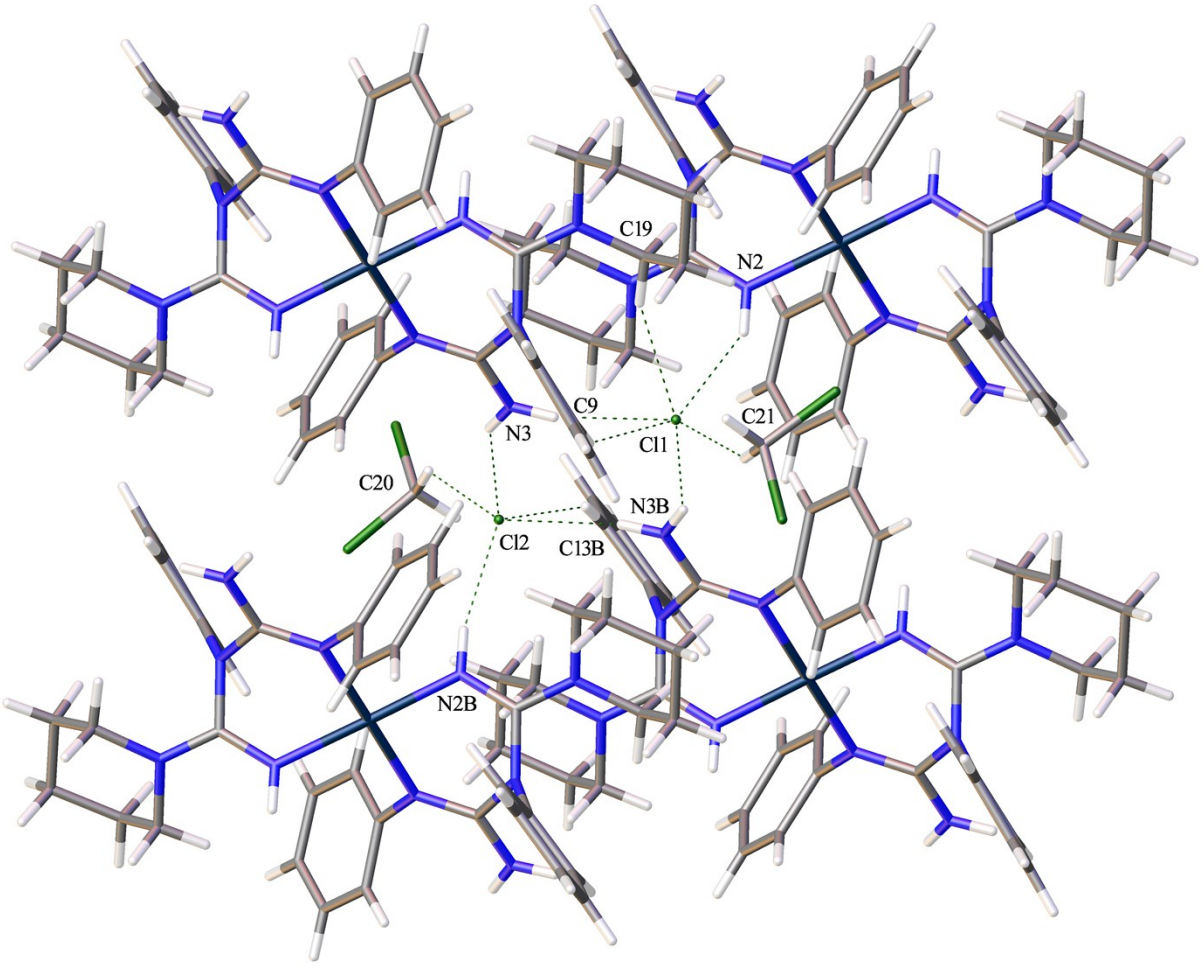

Figure S9. Intermolecular hydrogen bondings in the structure of [**1**][$Cl_2(CH_2Cl_2)_2$]showing the asymmetric environment of the Cl^- anions.

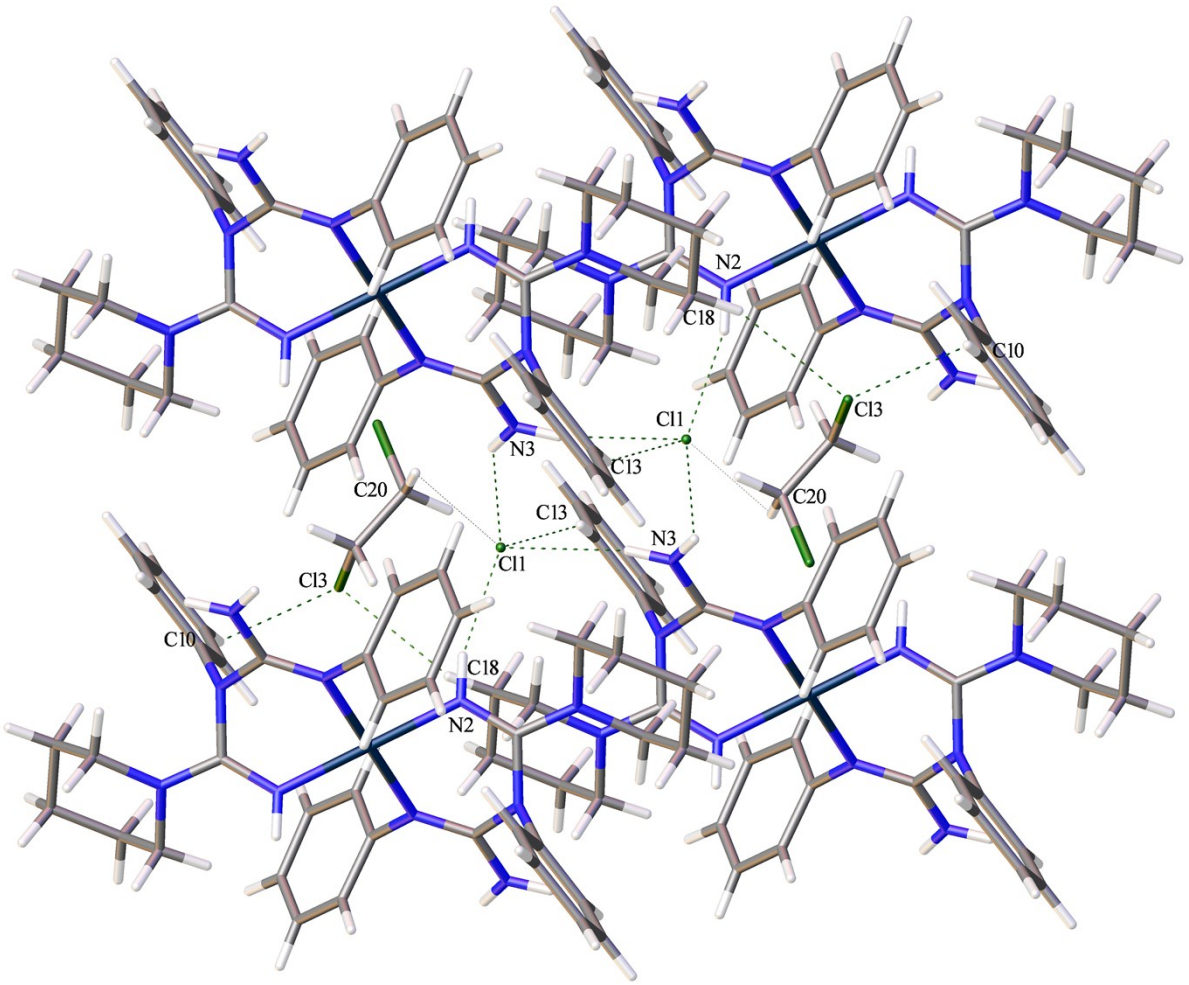

Figure S10. Intermolecular hydrogen bondings in the structure of [**1**][$Cl_2(C_2H_4Cl_2)_2$] showing the pyramidal environment of the Cl^- anions.

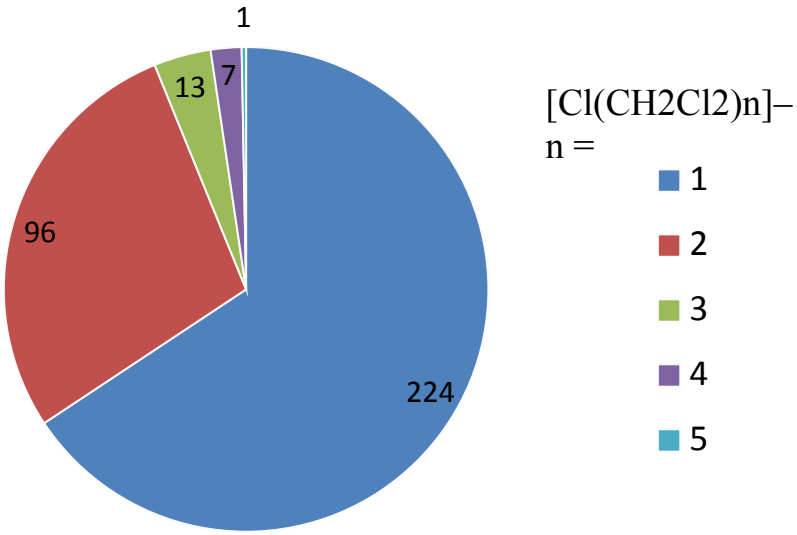

Figure S11. The distribution of the chloride-dichloromethane clusters $[Cl(CH_2Cl_2)_n]^-$ depending on the number of H-bonded chloroform molecules *n* (according to the CCDC database).

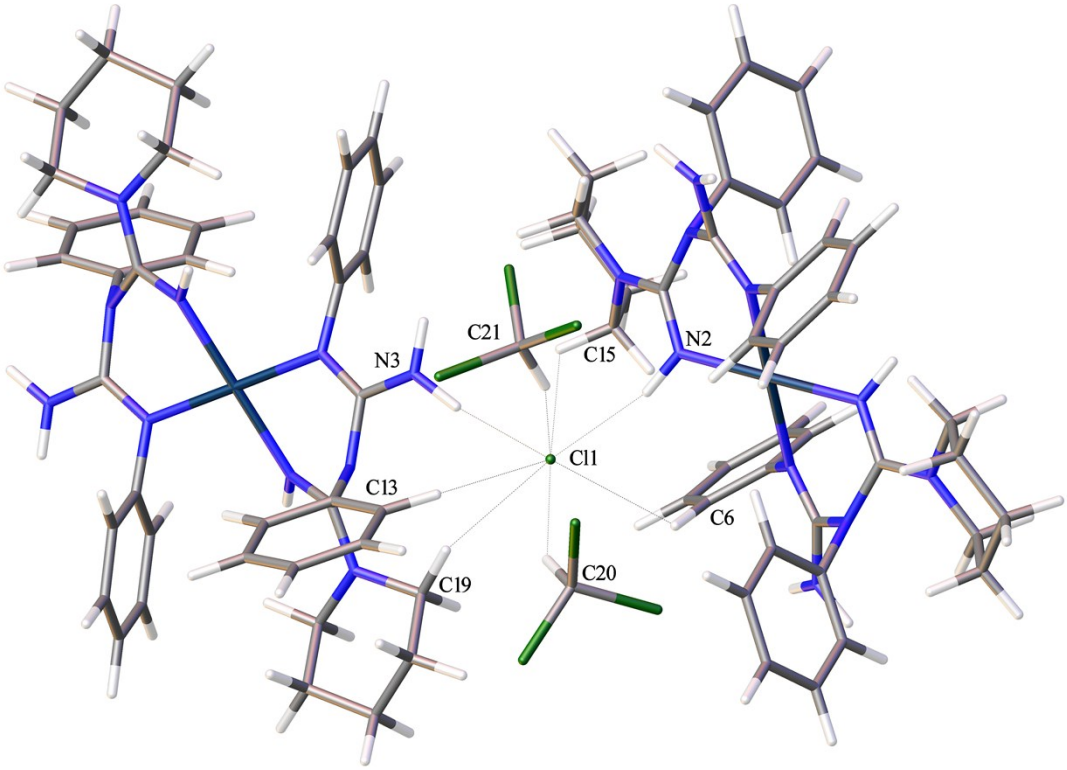

Figure S12. Graphical representation of hydrogen bondings formed by the Cl^- ion in the $[\mathbf{1}]_2[Cl(CHCl_3)_2]$ system according to DFT calculations.

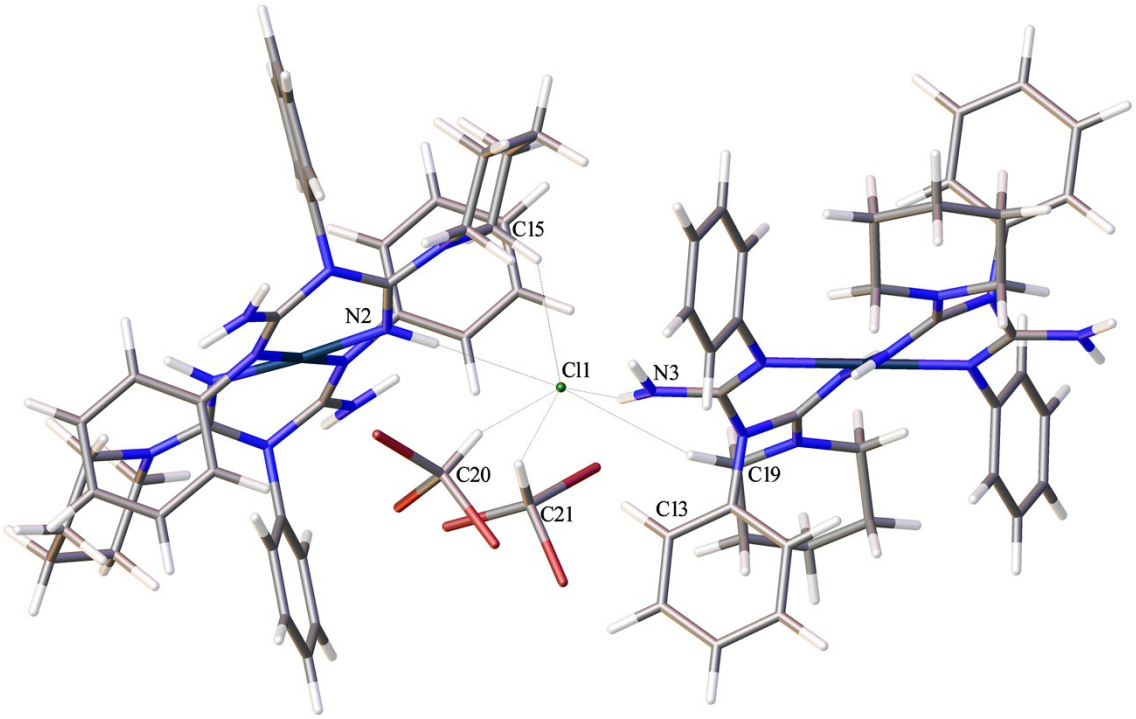

Figure S13. Graphical representation of hydrogen bondings formed by the Cl^- ion in the $[\mathbf{1}]_2[Cl(CHBr_3)_2]$ system according to DFT calculations.

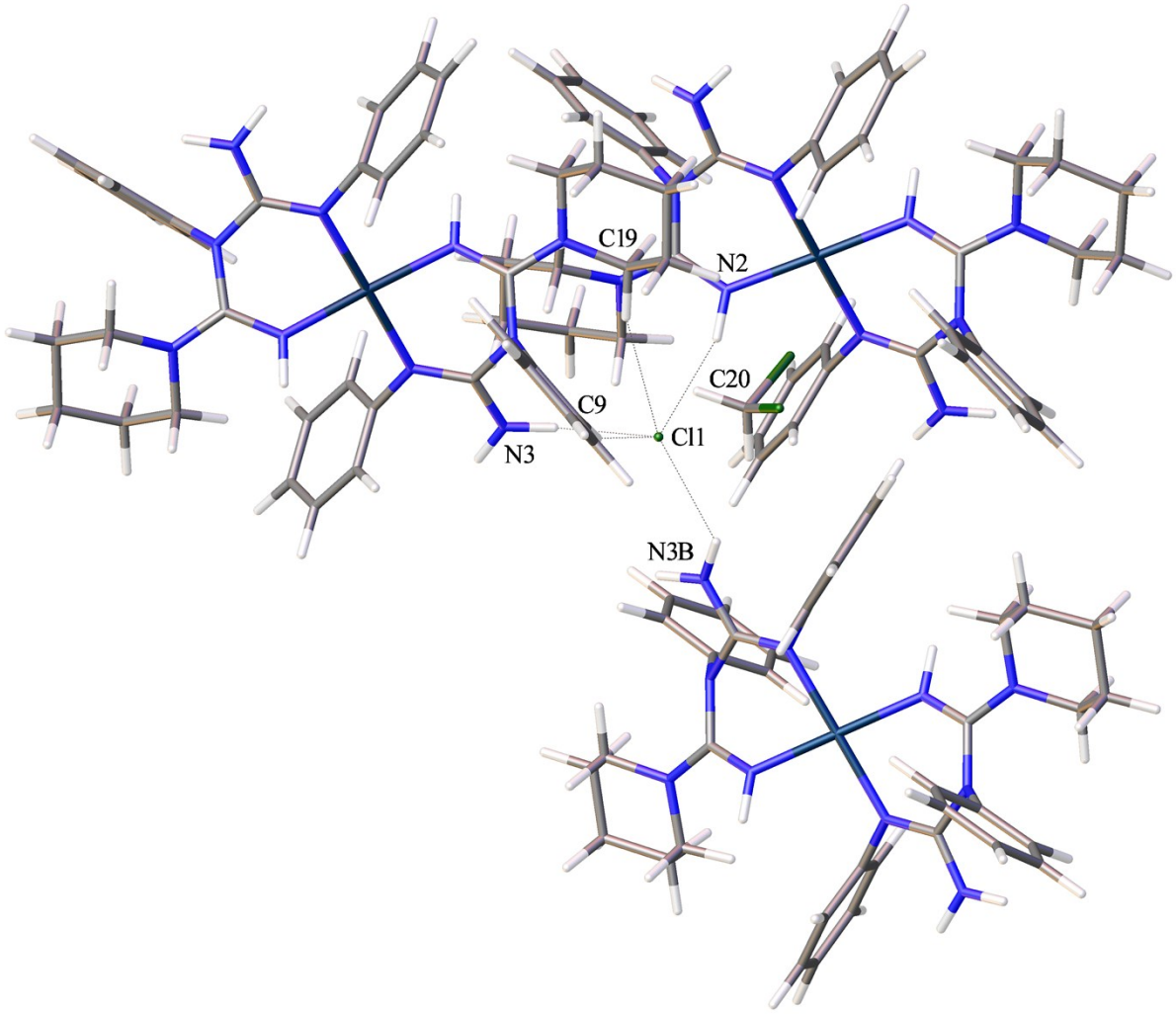

Figure S14. Graphical representation of hydrogen bondings formed by the Cl^- ion in the $[\mathbf{1}]_3[Cl(CH_2Cl_2)]$ system according to DFT calculations.

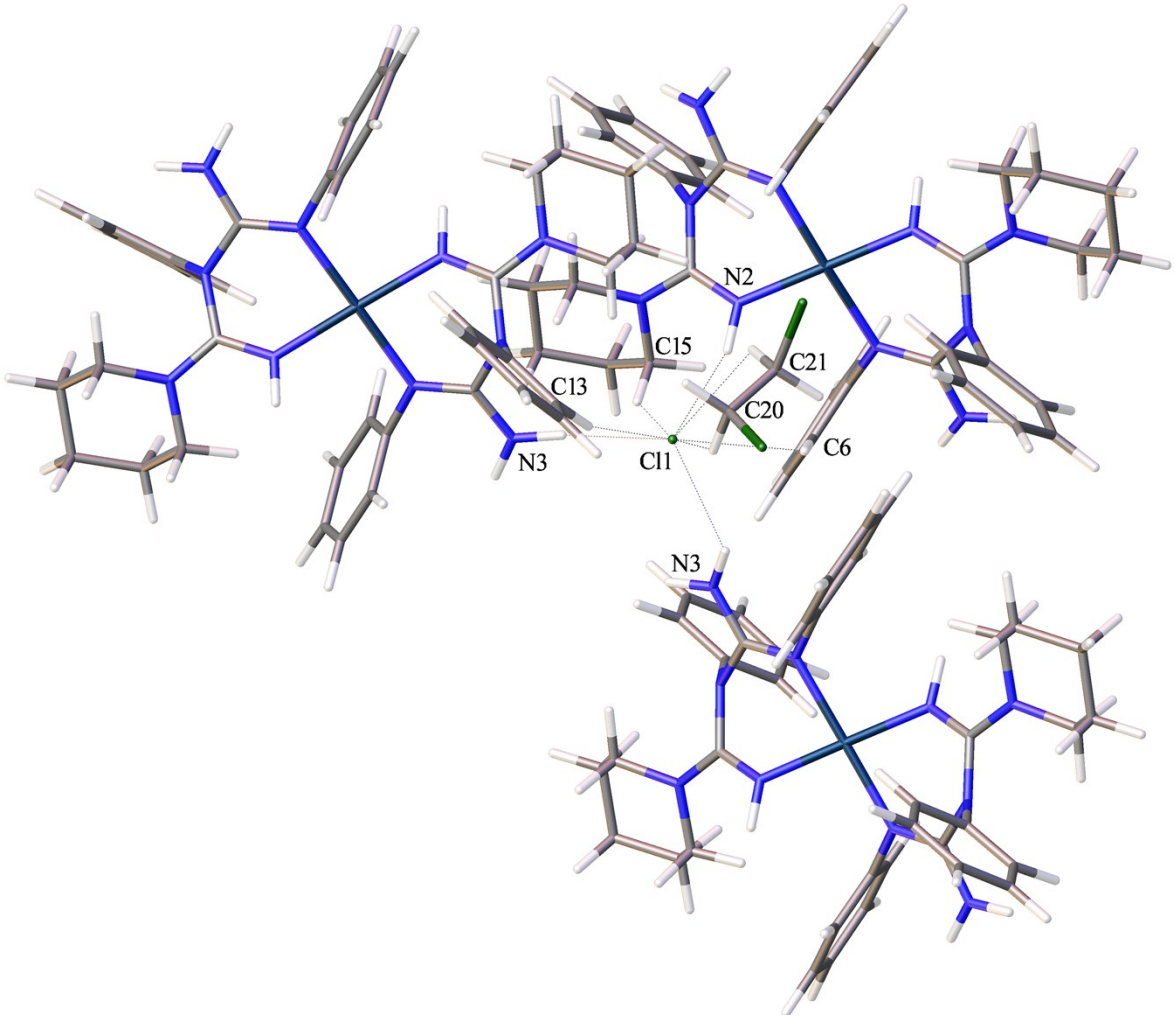

Figure S15. Graphical representation of hydrogen bondings formed by the Cl^- ion in the $[\mathbf{1}]_3[Cl(C_2H_4Cl_2)]$ system according to DFT calculations.

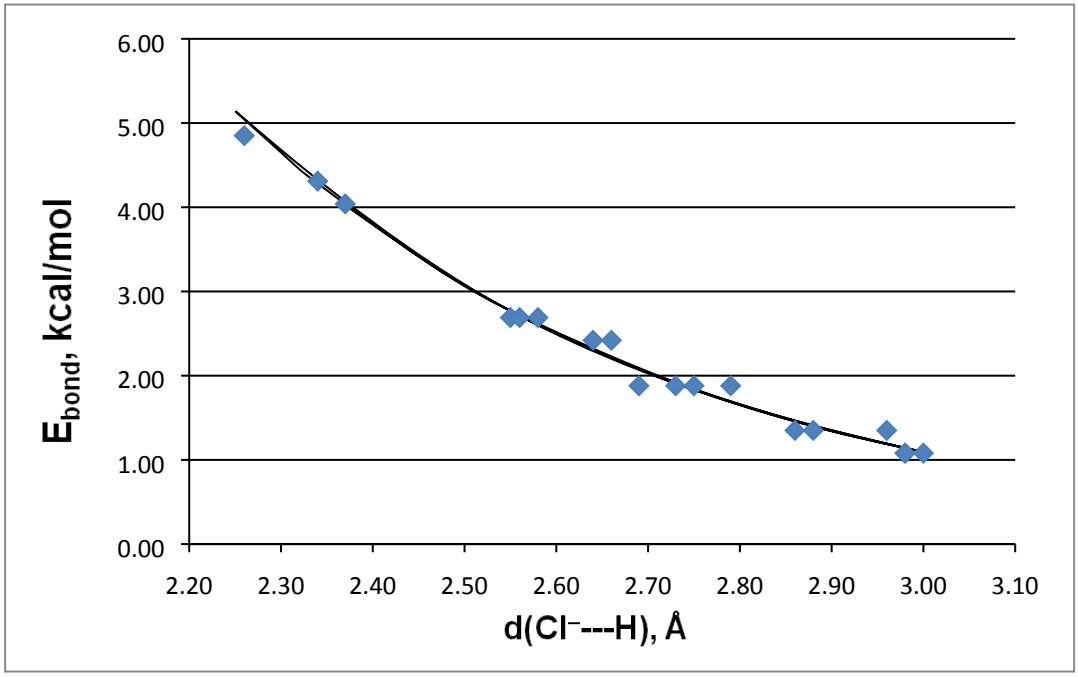

Figure S16. The correlation between theorethically calculated Cl⁻···H distances (Å) and energies of the corresponding contacts $E_{bond}{}^{b}$ (kcal/mol).

Table S3. Experimentally determined and theoretically calculated selected bond lengths, values of the density of all electrons – $\rho(\mathbf{r})$, Laplacian of electron density – $\nabla^2\rho(\mathbf{r})$, energy density – H_b, potential energy density – $V(\mathbf{r})$, and Lagrangian kinetic energy – $G(\mathbf{r})$ (Hartree) at the bond critical points (3, –1), corresponding to HBs in $[\mathbf{1}]_2[Cl(CHCl_3)_2]$, $[\mathbf{1}]_2[Cl(CHBr_3)_2]$, $[\mathbf{1}]_3[Cl(CH_2Cl_2)]$, and $[\mathbf{1}]_3[Cl(C_2H_4Cl_2)]$ as well as energies of these bonds E_{bond} (kcal/mol) defined bytwo methods.

Contact	Bond lengths, Å		$\rho(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$	H_b	V(r)	G(r)	E_{bond}[a]	E_{bond}[b]
	X-ray	Theory							
$[\mathbf{1}]_2[Cl(CHCl_3)_2]$									
$Cl^-\cdots H–C(20)Cl_3$	2.43	2.37	0.020	0.062	0.001	–0.014	0.015	4.39	4.04
$Cl^-\cdots H–C(21)Cl_3$	2.44	2.55	0.014	0.043	0.001	–0.009	0.010	2.82	2.69
$Cl^-\cdots H–N(3)H$	2.20	2.08	0.034	0.087	–0.003	–0.027	0.024	8.47	6.46
$Cl^-\cdots H–N(2)$	2.56	2.27	0.023	0.068	0.000	–0.017	0.017	5.33	4.58
$Cl^-\cdots H–C(19)H$	3.05	2.88	0.007	0.025	0.001	–0.004	0.005	1.26	1.35
$Cl^-\cdots H–C(15)H$	2.97	2.96	0.007	0.024	0.001	–0.004	0.005	1.26	1.35
$Cl^-\cdots H–C(13)$	2.73	2.56	0.014	0.044	0.001	–0.009	0.010	2.82	2.69
$Cl^-\cdots H–C(6)$	3.14	2.79	0.009	0.034	0.002	–0.005	0.007	1.57	1.88
$[\mathbf{1}]_2[Cl(CHBr_3)_2]$									
$Cl^-\cdots H–C(20)Br_3$	2.43	2.26	0.025	0.069	–0.001	–0.019	0.018	5.96	4.85
$Cl^-\cdots H–C(21)Br_3$	2.36	2.34	0.021	0.063	0.000	–0.015	0.016	4.71	4.31
$Cl^-\cdots H–N(3)H$	2.29	2.16	0.028	0.075	–0.001	–0.022	0.020	6.90	5.38
$Cl^-\cdots H–N(2)$	2.71	2.68	0.010	0.033	0.001	–0.006	0.007	1.88	1.88
$Cl^-\cdots H–C(15)H$	2.87	2.58	0.014	0.046	0.001	–0.009	0.010	2.82	2.69
$Cl^-\cdots H–C(19)H$	3.43	3.00	0.006	0.019	0.001	–0.003	0.004	0.94	1.08
$Cl^-\cdots H–C(13)$	2.83	2.86	0.008	0.025	0.001	–0.004	0.005	1.26	1.35
$[\mathbf{1}]_3[Cl(CH_2Cl_2)]$									
$Cl^-\cdots H–C(20)HCl_2$	2.58	2.98 3.00	Appropriate bond critical points (3, –1) were not found						

Cl⁻···H–N(3)H	2.40	2.24	0.024	0.066	–0.001	–0.018	0.017	5.65	4.58
Cl⁻···H–N(3B)H	2.45	2.52	0.014	0.047	0.001	–0.009	0.011	2.82	2.96
Cl⁻···H–N(2)	2.66	2.66	0.010	0.034	0.001	–0.006	0.007	1.88	1.88
Cl⁻···H–C(19)H	2.91	2.64	0.012	0.040	0.001	–0.007	0.009	2.20	2.42
Cl⁻···H–C(9)	2.79	2.69	0.011	0.035	0.001	–0.006	0.007	1.88	1.88
[**1**]$_3$[Cl($C_2H_4Cl_2$)]									
Cl⁻···H–C(20)H	2.83	2.73	0.010	0.035	0.002	–0.006	0.007	1.88	1.88
Cl⁻···H–C(21)H		2.98	0.006	0.021	0.001	–0.003	0.004	0.94	1.08
Cl⁻···H–N(3)H	2.57	2.30	0.021	0.060	0.000	–0.015	0.015	4.71	4.04
Cl⁻···H–N(3')H	2.52	2.59	0.011	0.040	0.001	–0.007	0.009	2.20	2.42
Cl⁻···H–N(2)	2.52	2.45	0.015	0.048	0.001	–0.010	0.011	3.14	2.96
Cl⁻···H–C(15)H	3.07	2.66	0.013	0.041	0.001	–0.008	0.009	2.51	2.42
Cl⁻···H–C(13)	2.82	2.75	0.011	0.034	0.001	–0.006	0.007	1.88	1.88
Cl⁻···H–C(6)		2.98	0.007	0.023	0.001	–0.003	0.004	0.94	1.08

[a] $E_{bond} = -V(\mathbf{r})/2$, see ref.[34] in the main text

[b] $E_{bond} = 0.429G(\mathbf{r})$, see ref. [35] in the main text

Table S4. Cartesian atomic coordinates of the calculated equilibrium structures.

Nuclear charges of elements are shown in the second column.

Structure	Charge	X	Y	Z
{[**1**]$_2$–($CHCl_3$)$_2$–Cl}	78	5.077307	-1.133332	0.627857
	7	5.125520	0.208747	2.178750
	7	7.100879	-0.926969	0.675583
	1	7.689867	-1.733314	0.485021
	7	5.812378	2.237254	3.076030
	7	7.066766	1.320127	1.361229
	1	6.574602	2.871278	3.262159
	1	5.004840	2.265754	3.686669
	7	9.043893	0.361115	0.559318
	6	4.133491	0.075956	3.206562
	6	4.289740	-0.915647	4.176070
	1	5.179458	-1.544657	4.159963
	6	3.312270	-1.078129	5.150532
	1	3.437546	-1.839740	5.917551
	6	2.180949	-0.262651	5.153029
	1	1.422174	-0.391738	5.922424
	6	2.026814	0.715103	4.175961
	1	1.138181	1.343463	4.156201
	6	3.003273	0.890235	3.197343
	1	2.872065	1.625513	2.402033
	6	5.962699	1.210888	2.222745
	6	7.198607	2.540559	0.574270
	6	6.763549	2.493992	-0.746835
	1	6.331569	1.568137	-1.131514
	6	6.872700	3.626285	-1.544575
	1	6.534974	3.595379	-2.578098
	6	7.392342	4.804034	-1.014220
	1	7.467461	5.693284	-1.635608
	6	7.815047	4.846666	0.310652
	1	8.226827	5.764383	0.724155
	6	7.732776	3.708843	1.106742
	1	8.117715	3.737027	2.126783
	6	7.745704	0.191401	0.867616
	6	9.732254	-0.521571	-0.391889
	1	8.989795	-1.110820	-0.943481
	1	10.379792	-1.217376	0.168046
	6	10.552222	0.309268	-1.370775
	1	9.855971	0.892285	-1.996326
	1	11.093171	-0.372899	-2.039910
	6	11.512640	1.247705	-0.652949
	1	12.267293	0.657170	-0.108567
	1	12.060818	1.861408	-1.377310
	6	10.749242	2.126770	0.329016
	1	11.433833	2.761611	0.905860
	1	10.063227	2.795050	-0.215720
	6	9.949743	1.262952	1.288528
	1	10.631124	0.625148	1.876987
	1	9.368144	1.851976	2.001397

	7	5.068354	-2.454149	-0.944568
	7	3.055731	-1.359778	0.605394
	1	2.442329	-0.565474	0.831065
	7	4.080185	-4.153263	-2.201536
	7	3.098041	-3.567897	-0.193386
	1	3.216666	-4.627478	-2.420666
	1	4.775390	-4.074593	-2.934084
	7	1.224350	-2.765852	0.957729
	6	6.126384	-2.311373	-1.900790
	6	6.284063	-1.103867	-2.582285
	1	5.555192	-0.308943	-2.424148
	6	7.365406	-0.932918	-3.437934
	1	7.485185	0.007880	-3.972477
	6	8.292099	-1.960142	-3.614209
	1	9.133390	-1.824232	-4.290378
	6	8.136767	-3.160385	-2.927604
	1	8.859848	-3.962614	-3.058407
	6	7.057381	-3.338832	-2.063981
	1	6.938791	-4.268810	-1.506750
	6	4.125244	-3.335189	-1.136558
	6	3.209334	-4.817585	0.547589
	6	3.765413	-4.765720	1.824309
	1	4.105932	-3.807111	2.221660
	6	3.873562	-5.932256	2.572488
	1	4.303069	-5.896056	3.571226
	6	3.445965	-7.144971	2.038725
	1	3.537335	-8.058478	2.621754
	6	2.901791	-7.190827	0.758749
	1	2.565046	-8.137179	0.341717
	6	2.773973	-6.024428	0.011394
	1	2.316766	-6.060837	-0.976761
	6	2.451369	-2.504350	0.459791
	6	0.690989	-2.015990	2.101350
	1	1.471385	-1.358937	2.499144
	1	-0.127236	-1.363362	1.749784
	6	0.213469	-2.986494	3.172272
	1	1.087698	-3.532835	3.563185
	1	-0.203446	-2.409873	4.008939
	6	-0.804263	-3.972586	2.618371
	1	-1.705782	-3.420947	2.297249
	1	-1.124068	-4.679672	3.393852
	6	-0.220187	-4.713310	1.421778
	1	-0.969580	-5.369076	0.957327
	1	0.617070	-5.352783	1.742606
	6	0.273070	-3.719215	0.382020
	1	-0.591097	-3.134044	0.006522
	1	0.733946	-4.211441	-0.479789
	17	3.160294	2.805569	-2.034991
	17	3.861470	3.679737	0.686350
	17	2.206096	5.386664	-1.025657
	6	2.626981	3.723316	-0.598675
	1	1.749571	3.199423	-0.205870
	78	-5.807392	0.649770	-0.139283
	7	-3.954018	-0.157842	-0.494917
	7	-4.803000	1.974219	1.038085

	1	-5.221493	2.314485	1.899963
	7	-1.664693	0.077619	-0.886792
	7	-2.870318	1.944977	-0.288606
	1	-0.808296	0.519877	-0.513889
	1	-1.583032	-0.895393	-1.158136
	7	-3.130981	3.584007	1.342284
	6	-3.852357	-1.574331	-0.656756
	6	-4.084571	-2.411496	0.435995
	1	-4.316295	-1.965726	1.403471
	6	-4.019819	-3.791903	0.273847
	1	-4.200854	-4.443897	1.126885
	6	-3.722399	-4.341191	-0.973171
	1	-3.674379	-5.421490	-1.095115
	6	-3.491906	-3.505085	-2.061834
	1	-3.264733	-3.927229	-3.038800
	6	-3.562240	-2.121304	-1.908738
	1	-3.385892	-1.456951	-2.756362
	6	-2.856658	0.564919	-0.552312
	6	-2.477657	2.863786	-1.351545
	6	-3.492284	3.619505	-1.939076
	1	-4.523206	3.487827	-1.605049
	6	-3.177199	4.540371	-2.930686
	1	-3.965682	5.134583	-3.387619
	6	-1.857176	4.688891	-3.349264
	1	-1.612484	5.403063	-4.132225
	6	-0.854258	3.922921	-2.764602
	1	0.181338	4.030384	-3.086319
	6	-1.156642	3.015932	-1.752662
	1	-0.362129	2.450003	-1.268091
	6	-3.638266	2.494203	0.743300
	6	-3.987527	4.578463	1.996524
	1	-5.037668	4.357135	1.769376
	1	-3.851263	4.509680	3.088982
	6	-3.629160	5.972569	1.496561
	1	-3.885407	6.032405	0.425964
	1	-4.255975	6.706260	2.020586
	6	-2.148764	6.273200	1.690532
	1	-1.918503	6.291816	2.768657
	1	-1.907619	7.269846	1.302156
	6	-1.299576	5.207634	1.007269
	1	-0.230240	5.368145	1.202083
	1	-1.436089	5.255904	-0.084375
	6	-1.686247	3.826043	1.506009
	1	-1.480210	3.753099	2.588079
	1	-1.121967	3.022618	1.020957
	7	-7.667269	1.457048	0.193348
	7	-6.787554	-0.667383	-1.329356
	1	-6.308381	-1.055797	-2.137397
	7	-9.977548	1.342003	0.401843
	7	-8.842451	-0.585817	-0.185472
	1	-10.835687	0.857447	0.187087
	1	-10.034198	2.303468	0.714394
	7	-8.369150	-2.345807	-1.649595
	6	-7.708075	2.862251	0.479410
	6	-7.466551	3.777666	-0.543676

	1	-7.306705	3.412075	-1.557737
	6	-7.430698	5.136509	-0.251850
	1	-7.251451	5.855526	-1.048640
	6	-7.636621	5.580792	1.053502
	1	-7.615928	6.645581	1.275391
	6	-7.881375	4.663059	2.071155
	1	-8.050246	5.007286	3.089400
	6	-7.913381	3.298400	1.789062
	1	-8.093767	2.565976	2.577549
	6	-8.787245	0.787520	0.127969
	6	-9.397839	-1.456207	0.846625
	6	-8.495401	-2.105476	1.685870
	1	-7.424452	-1.940248	1.550951
	6	-8.972824	-2.955178	2.676871
	1	-8.273693	-3.467933	3.333699
	6	-10.343554	-3.138450	2.837572
	1	-10.716452	-3.798318	3.617392
	6	-11.238903	-2.481839	1.999010
	1	-12.309614	-2.629726	2.118260
	6	-10.767527	-1.645734	0.991514
	1	-11.474570	-1.176314	0.306999
	6	-7.961493	-1.190318	-1.095650
	6	-7.403449	-3.344246	-2.128341
	1	-6.401644	-3.081468	-1.765893
	1	-7.384820	-3.331084	-3.231366
	6	-7.797708	-4.721862	-1.612784
	1	-7.699590	-4.717110	-0.514571
	1	-7.082654	-5.459302	-2.000891
	6	-9.224597	-5.077731	-2.005421
	1	-9.295210	-5.153599	-3.102685
	1	-9.499222	-6.061382	-1.606761
	6	-10.188879	-4.009554	-1.505233
	1	-11.212229	-4.212837	-1.845368
	1	-10.207253	-4.004133	-0.404052
	6	-9.765705	-2.641492	-2.011453
	1	-9.821764	-2.616974	-3.112940
	1	-10.405096	-1.836807	-1.640508
	17	0.613361	-1.894004	-2.344701
	17	2.999261	-0.721630	-3.552850
	17	0.439778	0.675808	-3.729067
	6	1.468755	-0.354649	-2.737652
	1	1.669771	0.150410	-1.780206
	17	0.932875	1.085300	0.471615
{[**1**]$_2$–(CHBr$_3$)$_2$–Cl}	78	5.241088	1.307337	0.743743
	7	5.348129	2.781617	-0.673464
	7	3.244474	1.674551	0.774325
	1	2.562441	0.934447	0.973667
	7	4.561631	4.690852	-1.738875
	1	3.861384	5.412667	-1.809756
	1	5.351757	4.718633	-2.371190
	7	1.529933	3.175002	1.244177
	7	3.438599	3.941361	0.143562
	6	6.387260	2.652211	-1.653134
	6	6.349678	1.599533	-2.567867

	1	5.507584	0.907818	-2.546893
	6	7.400185	1.436827	-3.463357
	1	7.370462	0.615502	-4.177473
	6	8.477159	2.322262	-3.458374
	1	9.288768	2.195845	-4.171705
	6	8.508848	3.372521	-2.545255
	1	9.346867	4.066413	-2.537790
	6	7.466662	3.537267	-1.634209
	1	7.484971	4.347191	-0.903051
	6	4.489175	3.757448	-0.775528
	6	3.508935	5.160583	0.936931
	6	3.019584	6.373026	0.463101
	1	2.527118	6.434268	-0.508262
	6	3.119107	7.510251	1.259412
	1	2.741451	8.461102	0.890351
	6	3.685454	7.426498	2.527322
	1	3.753274	8.315413	3.150130
	6	4.163146	6.207022	3.000143
	1	4.607285	6.141834	3.991017
	6	4.085426	5.071741	2.202244
	1	4.461055	4.108528	2.554664
	6	2.726846	2.867682	0.707849
	6	0.557876	4.060615	0.601640
	1	-0.236354	3.412689	0.185316
	1	1.039771	4.564781	-0.242681
	6	-0.042957	5.041700	1.595751
	1	0.735764	5.745006	1.929633
	1	-0.818111	5.632981	1.090074
	6	-0.611744	4.303621	2.801874
	1	-1.008547	5.016732	3.535103
	1	-1.458194	3.672249	2.480512
	6	0.462666	3.423902	3.426728
	1	0.067150	2.855937	4.279714
	1	1.282864	4.052964	3.810413
	6	1.020278	2.440143	2.411806
	1	1.849658	1.867247	2.842841
	1	0.256269	1.716212	2.086656
	7	5.189321	-0.167052	2.168653
	7	7.261525	1.023894	0.800882
	1	7.880070	1.821533	0.680647
	7	5.990576	-2.147585	3.101881
	1	6.821695	-2.683080	3.305412
	1	5.223588	-2.191962	3.762708
	7	9.137945	-0.361747	0.572646
	7	7.107486	-1.264278	1.277661
	6	4.185394	-0.059149	3.189011
	6	4.322228	0.894236	4.198302
	1	5.217927	1.514435	4.231628
	6	3.311473	1.032614	5.143697
	1	3.418346	1.765483	5.941065
	6	2.167748	0.235942	5.075723
	1	1.383221	0.351308	5.820970
	6	2.034975	-0.705131	4.060317
	1	1.148002	-1.330249	3.973940
	6	3.046231	-0.856114	3.116311

	1	2.960284	-1.593525	2.321120
	6	6.046860	-1.147024	2.206231
	6	7.028229	-2.313069	0.270335
	6	7.183990	-3.658634	0.587486
	1	7.395597	-3.974548	1.606974
	6	7.071418	-4.615131	-0.420128
	1	7.184013	-5.667755	-0.171310
	6	6.826487	-4.229725	-1.733945
	1	6.741287	-4.982930	-2.513480
	6	6.700122	-2.879367	-2.048038
	1	6.509658	-2.566873	-3.073540
	6	6.794907	-1.921037	-1.047911
	1	6.695057	-0.861593	-1.286576
	6	7.853369	-0.136218	0.891323
	6	9.933742	-1.476517	1.113408
	1	10.716953	-1.031310	1.749133
	1	9.294598	-2.085242	1.758347
	6	10.570918	-2.289058	-0.001160
	1	9.780812	-2.791979	-0.581048
	1	11.193957	-3.074519	0.445079
	6	11.398040	-1.385231	-0.906261
	1	11.828799	-1.958069	-1.735833
	1	12.246801	-0.973373	-0.336472
	6	10.541366	-0.243749	-1.435275
	1	11.136530	0.448494	-2.045327
	1	9.742900	-0.640639	-2.083803
	6	9.892590	0.544028	-0.303526
	1	9.214274	1.298326	-0.721935
	1	10.655092	1.066221	0.297162
	17	0.254849	-0.354746	0.550242
	6	2.047879	0.221543	-2.153769
	1	1.411823	0.334821	-1.266271
	35	2.628114	1.980633	-2.726591
	35	0.981881	-0.626885	-3.512212
	35	3.541726	-0.897624	-1.630094
	6	2.044890	-3.152161	0.476735
	1	1.834253	-2.075892	0.447935
	35	1.304086	-3.912294	-1.126982
	35	1.210201	-3.848399	2.076741
	35	3.956521	-3.455489	0.561406
	78	-6.449778	-0.416498	-0.150471
	7	-4.694899	0.502544	-0.683681
	7	-5.265484	-1.593325	1.014659
	1	-5.627113	-1.969205	1.886471
	7	-2.379322	0.488257	-1.009922
	1	-1.491544	0.110086	-0.638232
	1	-2.393820	1.468991	-1.262013
	7	-3.583502	-3.215123	1.131432
	7	-3.417461	-1.482993	-0.419192
	6	-4.759298	1.905091	-0.952448
	6	-5.028071	2.797648	0.086124
	1	-5.134163	2.411974	1.100089
	6	-5.163077	4.153512	-0.190092
	1	-5.371393	4.851336	0.618800
	6	-5.028936	4.622097	-1.496555

	1	-5.134813	5.684298	-1.707302
	6	-4.757712	3.730261	-2.529929
	1	-4.650943	4.091491	-3.550837
	6	-4.625912	2.368547	-2.262031
	1	-4.421500	1.656317	-3.062681
	6	-3.529910	-0.103076	-0.686897
	6	-3.072117	-2.316955	-1.563463
	6	-1.770552	-2.403509	-2.038531
	1	-0.952027	-1.880903	-1.541223
	6	-1.515181	-3.209163	-3.145284
	1	-0.496706	-3.274264	-3.528334
	6	-2.538476	-3.930713	-3.750613
	1	-2.324086	-4.563116	-4.609277
	6	-3.838155	-3.844081	-3.257043
	1	-4.641878	-4.403725	-3.730756
	6	-4.110235	-3.026138	-2.167571
	1	-5.124947	-2.931174	-1.774224
	6	-4.120283	-2.098107	0.619222
	6	-2.143330	-3.532992	1.115534
	1	-1.816963	-3.562546	2.169137
	1	-1.589560	-2.714047	0.646214
	6	-1.893773	-4.884828	0.464913
	1	-2.158338	-4.834482	-0.602998
	1	-0.820854	-5.106184	0.516796
	6	-2.708552	-5.966724	1.159977
	1	-2.563281	-6.937658	0.671078
	1	-2.353331	-6.082283	2.197918
	6	-4.182043	-5.589001	1.168643
	1	-4.785181	-6.332752	1.706534
	1	-4.561983	-5.546482	0.134136
	6	-4.401468	-4.226424	1.812309
	1	-5.460477	-3.951633	1.748375
	1	-4.119058	-4.249763	2.877658
	7	-8.214623	-1.332790	0.378659
	7	-7.624366	0.752510	-1.334723
	1	-7.248430	1.100980	-2.212904
	7	-10.512132	-1.344779	0.752979
	1	-11.405036	-0.951316	0.496027
	1	-10.493117	-2.308019	1.066063
	7	-9.379244	2.268550	-1.618525
	7	-9.535268	0.619667	0.025669
	6	-8.157570	-2.732944	0.684297
	6	-7.944141	-3.650597	-0.343618
	1	-7.858070	-3.290739	-1.368718
	6	-7.853138	-5.004934	-0.043114
	1	-7.699947	-5.726721	-0.842797
	6	-7.969589	-5.441648	1.275667
	1	-7.909336	-6.503614	1.503812
	6	-8.175426	-4.521046	2.298927
	1	-8.270837	-4.859420	3.328545
	6	-8.267012	-3.160716	2.007867
	1	-8.426746	-2.426713	2.799230
	6	-9.375611	-0.736073	0.375895
	6	-9.964011	1.524955	1.087116
	6	-11.294064	1.624594	1.479782

	1	-12.070907	1.039036	0.990059
	6	-11.644331	2.516036	2.488940
	1	-12.683530	2.593358	2.799633
	6	-10.674497	3.316915	3.083231
	1	-10.955635	4.018989	3.864643
	6	-9.346657	3.221240	2.676375
	1	-8.587589	3.846562	3.141281
	6	-8.985456	2.317903	1.683861
	1	-7.947462	2.226861	1.357469
	6	-8.808806	1.207166	-1.023147
	6	-10.831636	2.447004	-1.779807
	1	-11.045960	2.342582	-2.856863
	1	-11.348732	1.630332	-1.269462
	6	-11.278592	3.816327	-1.297021
	1	-11.134909	3.885037	-0.207543
	1	-12.353353	3.926667	-1.489390
	6	-10.482821	4.910232	-1.998237
	1	-10.769337	5.898134	-1.618895
	1	-10.719987	4.906902	-3.074622
	6	-8.990946	4.675555	-1.806910
	1	-8.398516	5.430316	-2.340958
	1	-8.733773	4.754303	-0.737296
	6	-8.575825	3.294197	-2.295474
	1	-7.515212	3.124086	-2.076823
	1	-8.721550	3.204874	-3.384994
{[**1**]$_3$–(CH_2Cl_2)–Cl}	78	-0.277196	4.415528	1.799741
	7	-2.067480	3.605164	2.397392
	7	-1.308307	6.171571	1.760854
	1	-0.814647	7.025469	2.009576
	7	-4.386878	3.402557	2.296614
	1	-4.330923	2.588313	2.898787
	1	-5.229739	3.955080	2.378461
	7	-3.101313	7.534688	1.133498
	7	-3.401161	5.224262	1.261954
	7	1.487561	5.245734	1.155583
	7	0.770316	2.678312	1.903806
	1	0.324385	1.782762	1.667403
	7	3.798593	5.505596	1.133116
	1	3.695828	6.459215	0.804155
	1	4.668997	5.289786	1.602650
	7	2.577579	1.381509	2.586424
	7	2.897949	3.663962	2.229549
	6	-2.020019	2.470714	3.277003
	6	-1.812796	2.676579	4.640221
	1	-1.700824	3.692048	5.018794
	6	-1.759393	1.580581	5.494569
	1	-1.611096	1.735971	6.561084
	6	-1.907541	0.290373	4.988302
	1	-1.876052	-0.563595	5.662120
	6	-2.096325	0.091686	3.623910
	1	-2.200669	-0.918238	3.225715
	6	-2.147487	1.182285	2.757724
	1	-2.260808	1.039978	1.680057
	6	-3.232152	4.055829	2.023754

	6	-4.025166	5.100934	-0.051574
	6	-5.395919	4.928086	-0.220350
	1	-6.071393	4.911038	0.633234
	6	-5.916757	4.822616	-1.507414
	1	-6.991327	4.709461	-1.641645
	6	-5.078475	4.905950	-2.616259
	1	-5.495821	4.845145	-3.619734
	6	-3.709466	5.091440	-2.440566
	1	-3.044304	5.148271	-3.300381
	6	-3.184023	5.193153	-1.158429
	1	-2.114705	5.348696	-1.009707
	6	-2.557693	6.343108	1.418931
	6	-4.528917	7.861027	1.307426
	1	-4.587877	8.584656	2.136875
	1	-5.062367	6.961836	1.627100
	6	-5.110976	8.474290	0.044890
	1	-6.155427	8.751179	0.236369
	1	-5.115290	7.721777	-0.759753
	6	-4.294195	9.689130	-0.379285
	1	-4.680739	10.104201	-1.317222
	1	-4.394935	10.483510	0.377280
	6	-2.827226	9.310324	-0.528918
	1	-2.216056	10.185427	-0.785880
	1	-2.707816	8.578931	-1.345925
	6	-2.275966	8.689772	0.748090
	1	-1.243835	8.359108	0.584501
	1	-2.278046	9.419347	1.573972
	6	1.364793	6.406662	0.319256
	6	1.575994	7.681086	0.849161
	1	1.861382	7.791900	1.897236
	6	1.415540	8.800977	0.033360
	1	1.589396	9.794350	0.442076
	6	1.033226	8.646878	-1.296489
	1	0.914667	9.521031	-1.932804
	6	0.808509	7.371687	-1.813148
	1	0.512434	7.251838	-2.853504
	6	0.971794	6.248343	-1.008933
	1	0.792147	5.243336	-1.394860
	6	2.681600	4.839332	1.499490
	6	3.856950	3.714864	3.325171
	6	3.351622	3.860550	4.614095
	1	2.272054	3.932342	4.760622
	6	4.228679	3.911317	5.691417
	1	3.839671	4.026583	6.700465
	6	5.603177	3.834679	5.477274
	1	6.287301	3.889022	6.320731
	6	6.102238	3.693327	4.186436
	1	7.175421	3.632446	4.020781
	6	5.228482	3.617618	3.104470
	1	5.617174	3.456986	2.096660
	6	2.027851	2.557224	2.203389
	6	1.763659	0.377351	3.287946
	1	1.356613	-0.347694	2.561732
	1	0.912976	0.897791	3.747983
	6	2.619643	-0.302922	4.345769

	1	2.910196	0.443120	5.102816
	1	2.015290	-1.064013	4.856289
	6	3.872199	-0.915408	3.732733
	1	3.581496	-1.692929	3.003622
	1	4.477762	-1.411667	4.501046
	6	4.680455	0.163609	3.023365
	1	5.052874	0.896377	3.756841
	1	5.557098	-0.264447	2.513243
	6	3.815051	0.867613	1.994809
	1	4.339840	1.689042	1.491705
	1	3.518594	0.142985	1.212715
	17	0.118922	-0.447319	0.237081
	17	-0.890347	2.732668	-1.082550
	17	-1.157714	2.057452	-3.952878
	6	-0.756815	1.456429	-2.328177
	1	0.276449	1.103860	-2.331182
	1	-1.441686	0.649860	-2.052839
	78	-6.612773	-3.039776	-0.196634
	7	-4.695180	-2.278256	-0.042928
	7	-5.731058	-4.821792	0.230945
	1	-6.174063	-5.675528	-0.102279
	7	-2.504248	-2.300561	0.758720
	1	-2.186160	-1.465267	0.265814
	1	-1.764978	-2.843893	1.180517
	7	-4.597488	-6.180761	1.748337
	7	-3.944272	-3.949141	1.487404
	7	-8.509632	-3.807922	-0.366456
	7	-7.501975	-1.265045	-0.597885
	1	-7.094662	-0.420125	-0.205661
	7	-10.639441	-3.926916	-1.278277
	1	-10.782601	-4.862209	-0.917369
	1	-11.378236	-3.514831	-1.829118
	7	-8.790825	0.180714	-1.879626
	7	-9.335146	-2.095939	-1.819326
	6	-4.421069	-1.089974	-0.793253
	6	-4.337510	-1.141549	-2.184179
	1	-4.411140	-2.106069	-2.685315
	6	-4.186809	0.037900	-2.908566
	1	-4.118404	0.000961	-3.994409
	6	-4.123267	1.264973	-2.248900
	1	-4.009422	2.188958	-2.815276
	6	-4.190893	1.311239	-0.858705
	1	-4.135340	2.271778	-0.345942
	6	-4.341047	0.135450	-0.127229
	1	-4.411214	0.156074	0.962793
	6	-3.738354	-2.813082	0.670896
	6	-3.821220	-3.691564	2.918169
	6	-2.598816	-3.781492	3.576791
	1	-1.697862	-4.074138	3.037312
	6	-2.541166	-3.537290	4.945773
	1	-1.591033	-3.626901	5.468833
	6	-3.698604	-3.212715	5.648642
	1	-3.653141	-3.044304	6.722468
	6	-4.917420	-3.119281	4.981918
	1	-5.822046	-2.869287	5.531676

	6	-4.980013	-3.352821	3.612550
	1	-5.927645	-3.288701	3.073814
	6	-4.787800	-5.011129	1.115688
	6	-3.288831	-6.687157	2.191682
	1	-3.033448	-7.530896	1.528292
	1	-2.535366	-5.912321	2.030282
	6	-3.347790	-7.170287	3.631687
	1	-2.367192	-7.575849	3.912517
	1	-3.550835	-6.315539	4.297318
	6	-4.437994	-8.223491	3.787648
	1	-4.515314	-8.547010	4.832008
	1	-4.171328	-9.118377	3.202707
	6	-5.770053	-7.673589	3.299494
	1	-6.558846	-8.435350	3.351402
	1	-6.089774	-6.836391	3.941983
	6	-5.681773	-7.169068	1.865932
	1	-6.627223	-6.695086	1.584468
	1	-5.489195	-8.000310	1.166926
	6	-8.793159	-5.016353	0.357580
	6	-8.773552	-6.243211	-0.310503
	1	-8.553478	-6.270902	-1.379327
	6	-9.061136	-7.413242	0.391128
	1	-9.065885	-8.367948	-0.130671
	6	-9.355584	-7.356223	1.750766
	1	-9.598079	-8.267365	2.293528
	6	-9.354976	-6.129885	2.414442
	1	-9.595806	-6.086065	3.474549
	6	-9.073240	-4.956276	1.721746
	1	-9.087560	-3.988400	2.222179
	6	-9.464493	-3.307574	-1.114593
	6	-9.675185	-2.120755	-3.240970
	6	-8.624854	-2.262955	-4.143372
	1	-7.603212	-2.354407	-3.768949
	6	-8.894467	-2.288494	-5.507179
	1	-8.080354	-2.401864	-6.219423
	6	-10.207177	-2.188227	-5.961184
	1	-10.417798	-2.218762	-7.027532
	6	-11.252219	-2.050030	-5.052710
	1	-12.277202	-1.966797	-5.406126
	6	-10.987931	-2.002733	-3.686835
	1	-11.806990	-1.841152	-2.983963
	6	-8.518833	-1.045085	-1.388797
	6	-7.726778	1.177193	-2.022534
	1	-7.813618	1.931189	-1.217894
	1	-6.756266	0.680678	-1.921822
	6	-7.824446	1.838915	-3.389066
	1	-7.632020	1.071128	-4.156874
	1	-7.020064	2.585016	-3.470713
	6	-9.198653	2.455600	-3.608119
	1	-9.361807	3.265051	-2.876166
	1	-9.266851	2.913570	-4.601774
	6	-10.277529	1.392629	-3.436546
	1	-10.186125	0.637530	-4.231788
	1	-11.279041	1.832242	-3.521507
	6	-10.147863	0.717685	-2.081869

	1	-10.874644	-0.084619	-1.937929
	1	-10.321105	1.454917	-1.278972
	78	6.927359	-1.573054	-1.229819
	7	8.729165	-0.794145	-1.826897
	7	7.762294	-3.355623	-1.680720
	1	7.155926	-4.096629	-2.022235
	7	11.040963	-0.794528	-2.006397
	1	11.062181	0.196199	-2.211400
	1	11.917593	-1.295019	-1.991743
	7	9.401755	-4.996629	-1.527048
	7	10.007420	-2.745496	-1.317610
	7	5.132445	-2.371360	-0.608469
	7	6.026274	0.225109	-0.812818
	1	6.592760	1.016863	-0.518602
	7	2.827331	-2.199883	-0.252029
	1	2.802696	-3.105837	0.200687
	1	1.999048	-1.590563	-0.166255
	7	4.351270	1.767052	-1.378105
	7	3.895175	-0.518786	-1.430007
	6	8.706831	0.543921	-2.339711
	6	8.288288	0.774486	-3.649769
	1	8.020381	-0.074114	-4.278837
	6	8.239026	2.077613	-4.134187
	1	7.934504	2.259743	-5.162896
	6	8.606226	3.146255	-3.317297
	1	8.589649	4.160719	-3.710249
	6	9.020019	2.912474	-2.008417
	1	9.325078	3.743339	-1.375300
	6	9.065620	1.610293	-1.512426
	1	9.398664	1.408360	-0.492725
	6	9.884355	-1.410564	-1.732834
	6	10.950287	-3.022598	-0.236317
	6	12.316129	-3.159325	-0.463434
	1	12.726776	-3.112093	-1.473287
	6	13.163873	-3.414489	0.610428
	1	14.232687	-3.519086	0.439746
	6	12.642193	-3.559098	1.892237
	1	13.307154	-3.771015	2.726089
	6	11.270919	-3.442433	2.107260
	1	10.864823	-3.562302	3.109190
	6	10.420276	-3.165090	1.043193
	1	9.341706	-3.069771	1.189191
	6	9.013450	-3.711844	-1.537269
	6	10.680476	-5.484470	-2.080197
	1	10.435089	-6.016475	-3.014645
	1	11.298433	-4.625666	-2.353120
	6	11.373379	-6.429749	-1.114081
	1	12.284787	-6.814641	-1.588460
	1	11.684831	-5.873935	-0.216108
	6	10.439857	-7.568120	-0.722965
	1	10.922803	-8.226681	0.007969
	1	10.221768	-8.189580	-1.606438
	6	9.140132	-7.009462	-0.161688
	1	8.434918	-7.812601	0.090370
	1	9.340440	-6.447703	0.766109

	6	8.467444	-6.067455	-1.150864
	1	7.578778	-5.617816	-0.692203
	1	8.154521	-6.612392	-2.057682
	6	5.196147	-3.607762	0.112028
	6	4.727519	-4.779735	-0.483016
	1	4.263062	-4.731886	-1.469126
	6	4.877405	-5.996318	0.180784
	1	4.516976	-6.912089	-0.283520
	6	5.496424	-6.041346	1.426656
	1	5.620122	-6.993259	1.938622
	6	5.957711	-4.866021	2.018350
	1	6.436668	-4.901441	2.994739
	6	5.808790	-3.647387	1.365371
	1	6.174477	-2.720171	1.808753
	6	3.989221	-1.747147	-0.730469
	6	3.318474	-0.563195	-2.766444
	6	4.167051	-0.327304	-3.848299
	1	5.227154	-0.130201	-3.675726
	6	3.652412	-0.334362	-5.139321
	1	4.311003	-0.147839	-5.984713
	6	2.300937	-0.594021	-5.349845
	1	1.900412	-0.605932	-6.360779
	6	1.466471	-0.840945	-4.264527
	1	0.408494	-1.040350	-4.426493
	6	1.965665	-0.820482	-2.964265
	1	1.300724	-0.986323	-2.115539
	6	4.804290	0.512505	-1.181581
	6	5.268383	2.885120	-1.624107
	1	5.255300	3.553708	-0.743055
	1	6.289335	2.507203	-1.750944
	6	4.853207	3.649986	-2.873039
	1	4.984344	2.987948	-3.744376
	1	5.539379	4.496182	-3.009067
	6	3.406991	4.110493	-2.782168
	1	3.304346	4.825306	-1.944477
	1	3.111758	4.647769	-3.691939
	6	2.495013	2.914610	-2.537488
	1	2.507482	2.240538	-3.409336
	1	1.453722	3.238927	-2.396696
	6	2.936385	2.160730	-1.292963
	1	2.315369	1.282049	-1.079401
	1	2.846173	2.834990	-0.418576
{[**1**]$_3$–($C_2H_4Cl_2$)–Cl}	78	6.962229	-1.495386	-1.203450
	7	5.070885	-2.235552	-0.846944
	7	2.753646	-1.938136	-0.692147
	1	2.624575	-2.883789	-0.354005
	1	1.962702	-1.282977	-0.626232
	7	4.036493	-0.225272	-1.563849
	7	4.576972	1.998731	-1.159066
	7	6.136419	0.308951	-0.675718
	1	6.712946	1.019695	-0.231693
	6	4.986112	-3.555570	-0.299371
	6	4.473414	-4.594902	-1.077427
	1	4.091088	-4.380309	-2.076370

	6	4.476039	-5.896005	-0.577944
	1	4.083804	-6.707482	-1.187538
	6	4.993840	-6.157963	0.687116
	1	5.004203	-7.175507	1.071742
	6	5.505804	-5.115845	1.459419
	1	5.911541	-5.320342	2.448249
	6	5.505012	-3.814588	0.970161
	1	5.914509	-2.991119	1.556151
	6	3.985909	-1.523236	-1.005481
	6	3.609656	-0.090609	-2.951334
	6	2.268148	-0.188856	-3.305727
	1	1.502381	-0.344327	-2.544329
	6	1.913551	-0.056748	-4.646389
	1	0.866692	-0.141419	-4.935363
	6	2.881270	0.196097	-5.613670
	1	2.593506	0.305434	-6.656648
	6	4.219176	0.306334	-5.245480
	1	4.979191	0.496509	-6.000086
	6	4.589668	0.151117	-3.914675
	1	5.638974	0.217186	-3.620182
	6	4.967223	0.710895	-1.104196
	6	3.170538	2.429291	-1.185608
	1	2.998385	3.007144	-0.256028
	1	2.513148	1.552906	-1.147977
	6	2.892936	3.323681	-2.381340
	1	2.993489	2.738839	-3.309717
	1	1.848319	3.665968	-2.332636
	6	3.855918	4.504751	-2.392424
	1	3.673314	5.131641	-1.500418
	1	3.680102	5.142423	-3.267514
	6	5.293530	4.007986	-2.364819
	1	5.511941	3.430137	-3.277669
	1	6.007941	4.841009	-2.333632
	6	5.536869	3.106868	-1.161637
	1	6.560988	2.717774	-1.191609
	1	5.413120	3.677054	-0.222046
	7	8.855148	-0.779796	-1.531262
	7	11.169534	-0.930926	-1.500991
	1	11.276679	0.070512	-1.600257
	1	12.004627	-1.497733	-1.478586
	7	9.955045	-2.859487	-1.116046
	7	9.246933	-5.032704	-1.619713
	7	7.733280	-3.273569	-1.774646
	1	7.125082	-3.930561	-2.256030
	6	8.963046	0.606394	-1.878717
	6	9.290816	1.540891	-0.893684
	1	9.505460	1.196967	0.119787
	6	9.366484	2.892877	-1.224751
	1	9.649223	3.619951	-0.466058
	6	9.102833	3.307352	-2.527850
	1	9.179593	4.360298	-2.790607
	6	8.767299	2.369631	-3.503715
	1	8.581358	2.692017	-4.526215
	6	8.697681	1.017418	-3.184224
	1	8.453942	0.270271	-3.939084

	6	9.954900	-1.484025	-1.401295
	6	10.739583	-3.288606	0.039757
	6	12.110610	-3.510007	-0.036712
	1	12.643656	-3.416678	-0.984177
	6	12.802284	-3.908392	1.103455
	1	13.874723	-4.079590	1.049402
	6	12.121030	-4.106278	2.300644
	1	12.665321	-4.426213	3.186003
	6	10.745351	-3.899987	2.364158
	1	10.214931	-4.058408	3.300521
	6	10.050868	-3.482186	1.234540
	1	8.972930	-3.309333	1.265537
	6	8.937560	-3.729285	-1.537244
	6	10.552075	-5.555197	-2.070441
	1	10.388237	-5.982235	-3.073978
	1	11.247166	-4.721481	-2.189487
	6	11.069886	-6.629210	-1.129987
	1	11.298028	-6.180148	-0.151123
	1	12.010482	-7.027413	-1.530782
	6	10.034786	-7.734881	-0.965458
	1	9.895420	-8.257957	-1.925152
	1	10.386878	-8.486476	-0.249579
	6	8.707701	-7.143020	-0.510947
	1	8.823651	-6.681152	0.484034
	1	7.934787	-7.918293	-0.423101
	6	8.216354	-6.071009	-1.474165
	1	7.297903	-5.614394	-1.086282
	1	7.998028	-6.504951	-2.464455
	17	0.049982	-0.063063	-0.226966
	17	-1.839315	1.950461	-4.518435
	17	-0.686755	4.530446	-2.738661
	6	-0.751025	1.809437	-3.095832
	1	-0.926151	0.835003	-2.620918
	1	0.277711	1.846368	-3.474358
	6	-0.988195	2.878784	-2.069957
	1	-0.300172	2.726846	-1.226154
	1	-2.018925	2.867057	-1.694063
	78	-6.519574	-3.180550	-0.078288
	7	-8.375471	-4.052932	-0.063136
	7	-10.598858	-4.217774	-0.713425
	1	-10.687782	-5.153256	-0.335748
	1	-11.412055	-3.796572	-1.138002
	7	-9.408487	-2.358597	-1.394184
	7	-8.999245	-0.058851	-1.463486
	7	-7.546988	-1.443714	-0.284541
	1	-7.149398	-0.585546	0.087972
	6	-8.511532	-5.286678	0.660178
	6	-8.564754	-6.494413	-0.039583
	1	-8.532703	-6.487037	-1.130461
	6	-8.677065	-7.692423	0.664117
	1	-8.737136	-8.633404	0.121268
	6	-8.724102	-7.682046	2.055684
	1	-8.827940	-8.616955	2.602264
	6	-8.654796	-6.473494	2.747799
	1	-8.705575	-6.466101	3.834556

	6	-8.547720	-5.271934	2.053771
	1	-8.509005	-4.317958	2.579356
	6	-9.426728	-3.574056	-0.682298
	6	-9.755014	-2.433990	-2.812663
	6	-11.074937	-2.431807	-3.250324
	1	-11.901840	-2.327862	-2.546294
	6	-11.341111	-2.517635	-4.613915
	1	-12.371352	-2.522822	-4.961671
	6	-10.293052	-2.579701	-5.527490
	1	-10.506373	-2.639975	-6.592055
	6	-8.973961	-2.562826	-5.081268
	1	-8.156800	-2.613994	-5.797275
	6	-8.700192	-2.497762	-3.719673
	1	-7.672492	-2.494216	-3.349298
	6	-8.623985	-1.267601	-1.006745
	6	-10.399078	0.370268	-1.633527
	1	-10.609773	1.092188	-0.826181
	1	-11.054490	-0.489259	-1.474724
	6	-10.618456	1.028349	-2.984673
	1	-10.500405	0.278456	-3.781668
	1	-11.651835	1.393062	-3.036559
	6	-9.626913	2.166939	-3.193670
	1	-9.825583	2.968566	-2.462050
	1	-9.756989	2.610950	-4.187542
	6	-8.204612	1.656492	-3.012666
	1	-7.974744	0.900974	-3.782556
	1	-7.465234	2.463304	-3.121221
	6	-8.015081	1.011863	-1.647399
	1	-7.007515	0.587707	-1.576711
	1	-8.131387	1.759326	-0.841855
	7	-4.645037	-2.316049	-0.103915
	7	-2.367417	-2.251973	0.389329
	1	-2.179182	-1.371427	-0.089962
	1	-1.545333	-2.781570	0.638223
	7	-3.608352	-4.033523	1.186561
	7	-4.086891	-6.315299	1.347164
	7	-5.503392	-4.930462	0.118383
	1	-5.938342	-5.785953	-0.220672
	6	-4.519080	-1.085109	-0.824639
	6	-4.467154	0.117246	-0.118862
	1	-4.467037	0.095823	0.973467
	6	-4.416982	1.322590	-0.817666
	1	-4.394650	2.268061	-0.272353
	6	-4.418398	1.321591	-2.209438
	1	-4.384172	2.263560	-2.755116
	6	-4.465685	0.115534	-2.908262
	1	-4.450851	0.119822	-3.996092
	6	-4.521322	-1.090711	-2.219033
	1	-4.570636	-2.042074	-2.748267
	6	-3.574798	-2.836096	0.435332
	6	-3.316616	-3.884815	2.607468
	6	-2.011077	-3.858335	3.087162
	1	-1.167283	-3.978715	2.408133
	6	-1.785142	-3.719894	4.453814
	1	-0.765487	-3.715506	4.833753

	6	-2.859000	-3.627270	5.335068
	1	-2.680299	-3.544154	6.405084
	6	-4.163609	-3.663060	4.849387
	1	-5.003576	-3.599852	5.537418
	6	-4.395605	-3.786435	3.483901
	1	-5.413772	-3.824216	3.091367
	6	-4.433209	-5.119300	0.842290
	6	-2.699521	-6.766391	1.539147
	1	-2.504052	-7.528276	0.765255
	1	-2.024611	-5.928400	1.343544
	6	-2.499474	-7.374487	2.917321
	1	-2.613405	-6.592302	3.684108
	1	-1.472259	-7.754355	2.991458
	6	-3.510630	-8.488940	3.159493
	1	-3.317347	-9.320812	2.463210
	1	-3.398876	-8.897591	4.170388
	6	-4.923555	-7.966173	2.945492
	1	-5.152453	-7.181111	3.685880
	1	-5.667964	-8.761868	3.077702
	6	-5.092383	-7.369428	1.556167
	1	-6.092052	-6.931917	1.459112
	1	-4.975415	-8.142023	0.777609
	78	-0.364280	4.393602	1.688472
	7	-2.155321	3.532445	2.217384
	7	-4.473180	3.376019	2.335269
	1	-4.385991	2.535476	2.894543
	1	-5.316583	3.917202	2.464217
	7	-3.559024	5.219643	1.279806
	7	-3.184755	7.507738	1.016197
	7	-1.417199	6.131573	1.655990
	1	-0.912093	6.997404	1.838082
	6	-2.079025	2.353811	3.036421
	6	-2.158223	1.097610	2.438334
	1	-2.236638	1.020178	1.350868
	6	-2.095748	-0.043138	3.236855
	1	-2.154395	-1.029285	2.773294
	6	-1.945718	0.074358	4.615799
	1	-1.906022	-0.820987	5.234282
	6	-1.849582	1.334995	5.203305
	1	-1.733786	1.429293	6.280963
	6	-1.914820	2.480216	4.416014
	1	-1.844608	3.473292	4.859572
	6	-3.340767	4.024755	1.979722
	6	-4.364057	5.133192	0.063900
	6	-5.753661	5.076849	0.085141
	1	-6.307250	5.134728	1.021884
	6	-6.450226	4.999237	-1.118700
	1	-7.538141	4.970070	-1.107406
	6	-5.764528	5.004189	-2.330656
	1	-6.317231	4.978541	-3.267836
	6	-4.373019	5.076412	-2.343824
	1	-3.825190	5.092812	-3.285434
	6	-3.672551	5.135063	-1.144489
	1	-2.583136	5.212034	-1.147801
	6	-2.673255	6.311594	1.347055

	6	-4.541917	7.950929	1.387895
	1	-4.423708	8.679398	2.207779
	1	-5.093925	7.098837	1.794284
	6	-5.248753	8.606441	0.216021
	1	-5.430617	7.854191	-0.568033
	1	-6.227728	8.970549	0.552204
	6	-4.403540	9.747140	-0.338344
	1	-4.317021	10.543676	0.418073
	1	-4.889880	10.199495	-1.210150
	6	-3.016956	9.239041	-0.706978
	1	-3.093563	8.501301	-1.522119
	1	-2.377236	10.054474	-1.068885
	6	-2.326660	8.573952	0.476108
	1	-1.376896	8.130024	0.153302
	1	-2.113554	9.309547	1.270888
	7	1.452508	5.291651	1.316338
	7	3.733362	5.582790	1.660339
	1	3.649785	6.567647	1.433298
	1	4.540667	5.321377	2.211832
	7	2.751460	3.613137	2.399499
	7	2.432472	1.306424	2.479720
	7	0.691513	2.661015	1.735001
	1	0.283375	1.793701	1.356949
	6	1.428859	6.570193	0.659337
	6	1.439722	7.745036	1.416276
	1	1.502183	7.686605	2.504986
	6	1.376398	8.978019	0.768044
	1	1.394010	9.895710	1.352436
	6	1.293728	9.033437	-0.621576
	1	1.248774	9.997186	-1.124219
	6	1.276640	7.855950	-1.366685
	1	1.212846	7.897645	-2.452305
	6	1.344574	6.621582	-0.728138
	1	1.317572	5.691066	-1.293298
	6	2.597774	4.862132	1.781843
	6	3.545834	3.553083	3.620168
	6	4.936417	3.492576	3.591062
	1	5.468599	3.452306	2.638438
	6	5.644466	3.454941	4.790270
	1	6.731398	3.423649	4.775659
	6	4.962577	3.448312	6.002854
	1	5.517924	3.417030	6.937245
	6	3.570072	3.487450	6.022109
	1	3.038814	3.486517	6.971118
	6	2.857406	3.548057	4.830627
	1	1.766083	3.589604	4.828082
	6	1.908684	2.514080	2.159330
	6	3.730843	0.859313	1.970845
	1	3.522464	0.234339	1.080070
	1	4.304149	1.730754	1.630151
	6	4.483778	0.036154	2.999073
	1	4.766673	0.679843	3.847435
	1	5.413239	-0.335684	2.541754
	6	3.614172	-1.114829	3.489858
	1	3.412127	-1.803450	2.648665

	1	4.138708	-1.695762	4.258396
	6	2.295461	-0.572724	4.026091
	1	2.490083	0.077470	4.893963
	1	1.639470	-1.384141	4.370489
	6	1.561317	0.228323	2.962665
	1	0.653949	0.686925	3.375062
	1	1.254668	-0.411008	2.116386

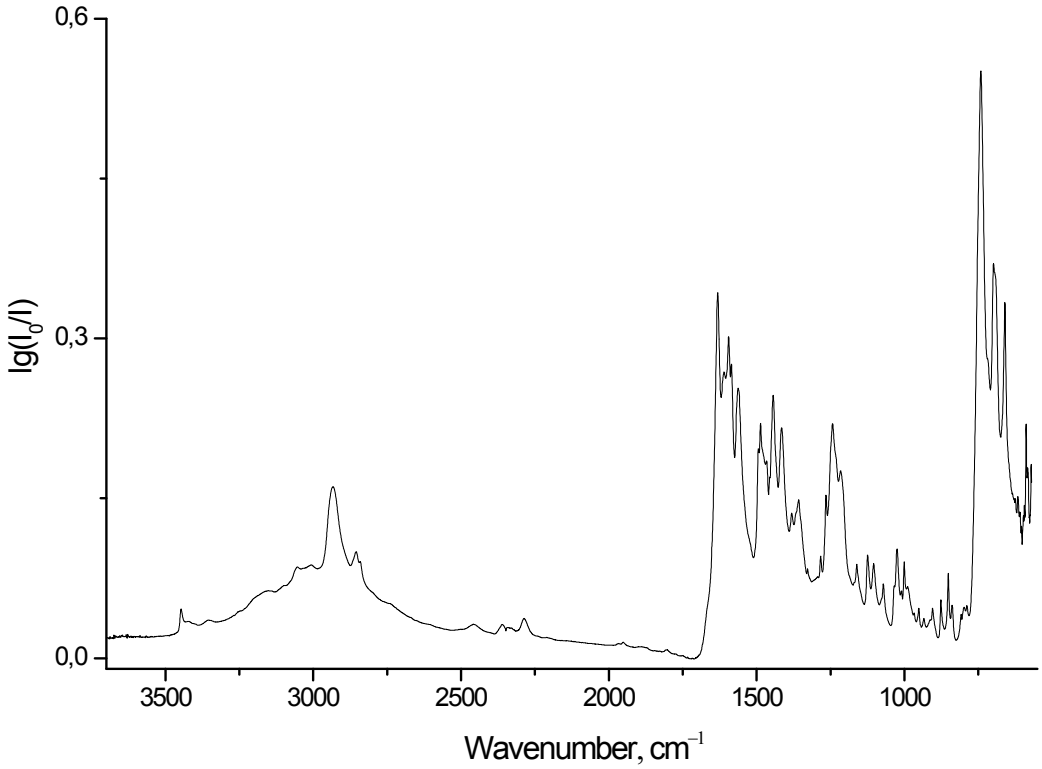

Figure S17. ATR IR spectrum of [**1**][$Cl_2(CHCl_3)_4$].

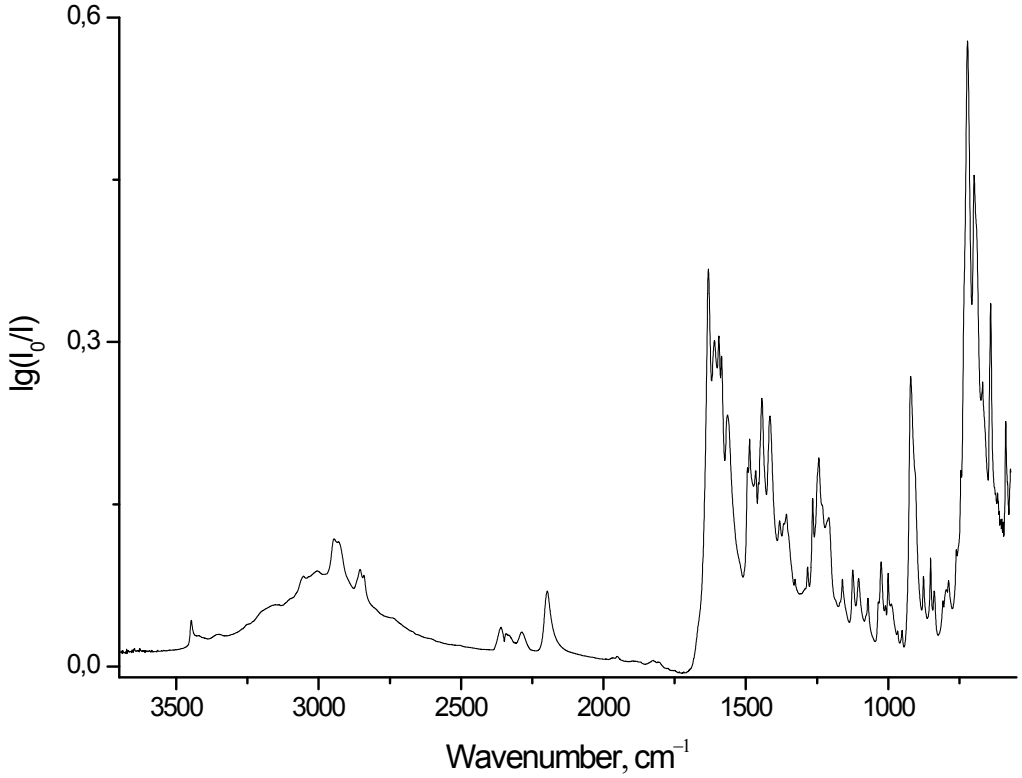

Figure S18. ATR IR spectrum of [**1**][$Cl_2(CDCl_3)_4$].

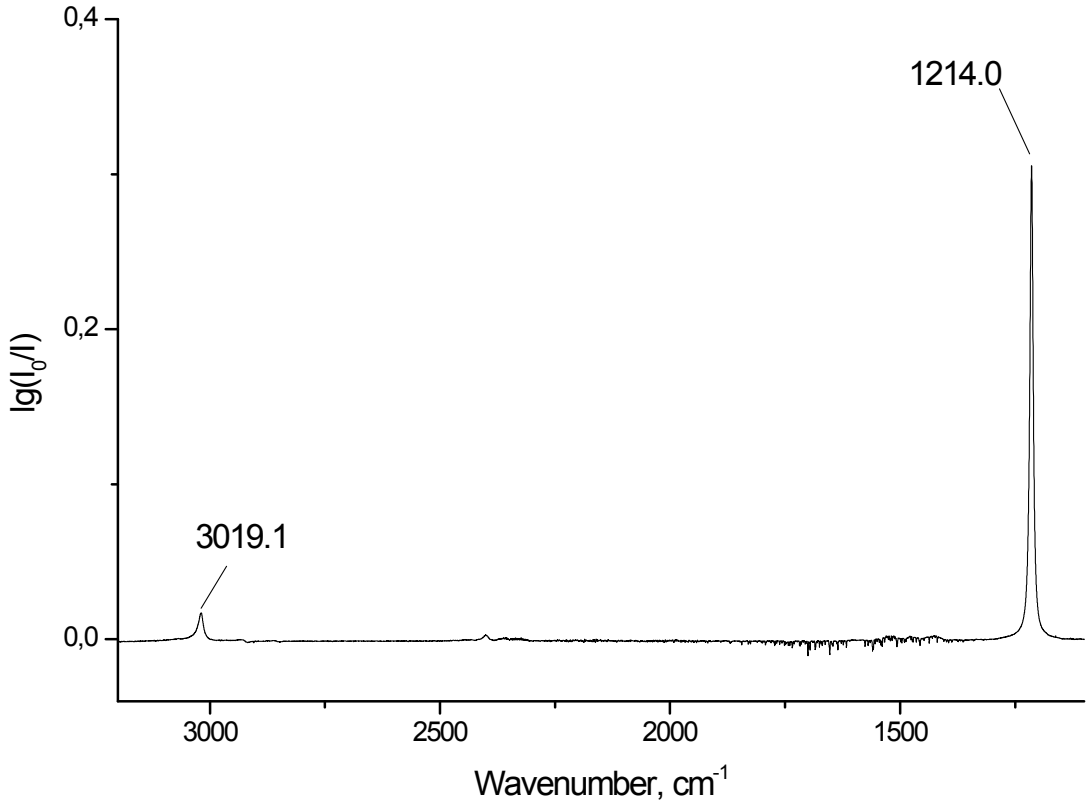

Figure S19. ATR IR spectrum of neat $CHCl_3$.

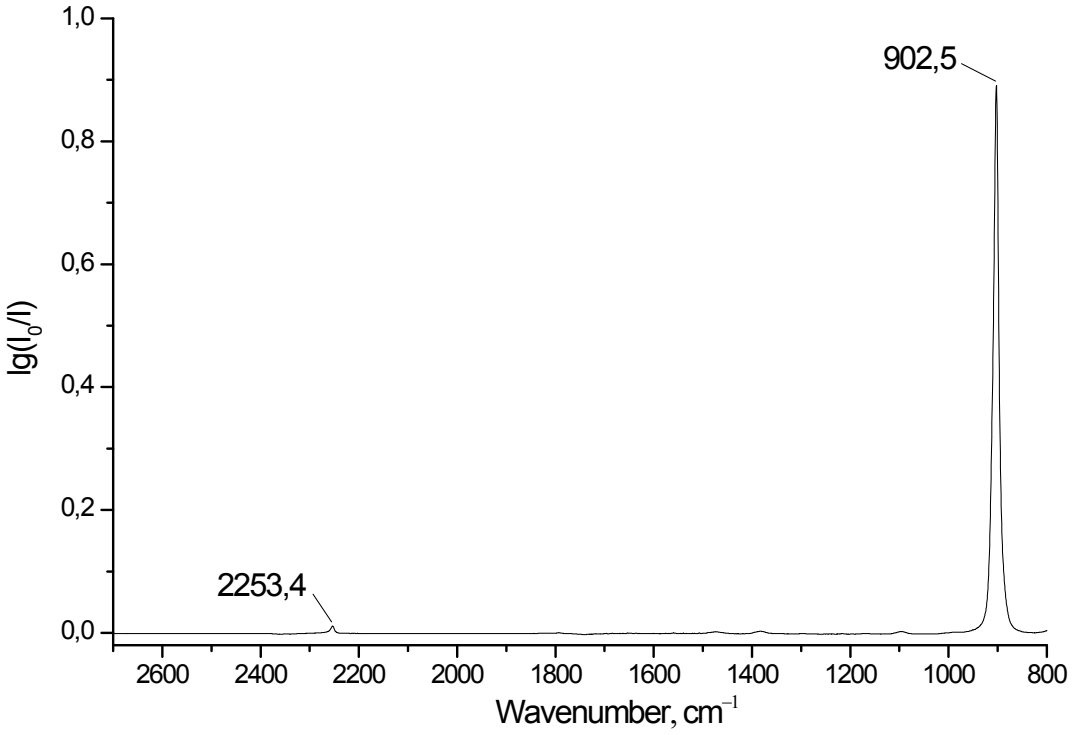

Figure S20. ATR IR spectrum of neat $CDCl_3$.

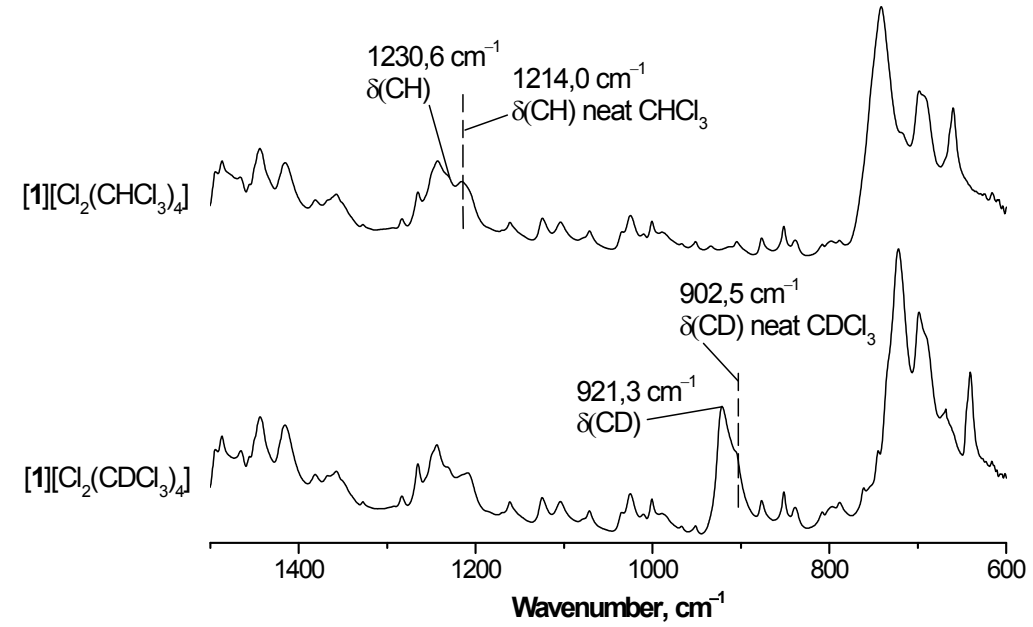

Figure S21. ATR FTIR spectra of [**1**][$Cl_2(CHCl_3)_4$] and [**1**][$Cl_2(CDCl_3)_4$] in the range 1500–600 cm^{-1}.

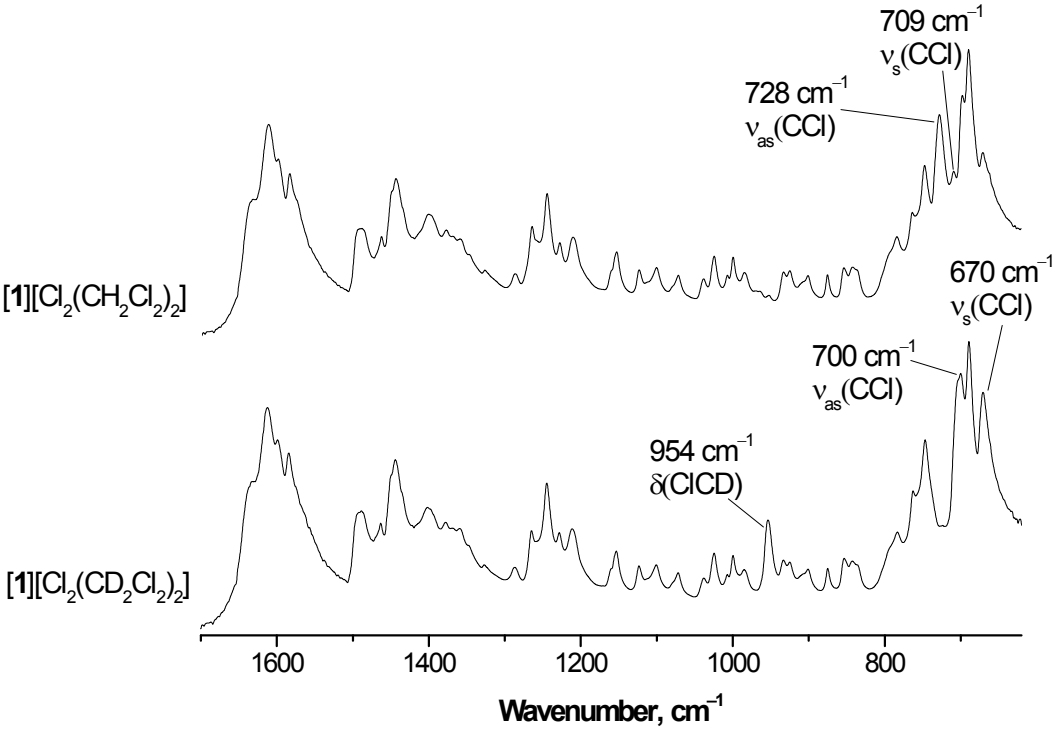

Figure S22. ATR FTIR spectra of [**1**][$Cl_2(CH_2Cl_2)_2$] and [**1**][$Cl_2(CD_2Cl_2)_2$] in the range 1700–600 cm^{-1}.

Table S5. Crystallographic parameters of C–H···Cl^- hydrogen bonds formed between chloride anion and co-crystallized 1,2-dichloroethane molecules (according to CCDC database).

Compound	*d*(H···A), Å	*d*(D···A), Å	∠(DHA), deg	Ref.
$[(C_{65}H_{54}OsO_3P_3S)Cl]\cdot 2½C_2H_4Cl_2\cdot H_2O$	2.81	3.581	137.2	[1]
$[(C_{30}H_{42}PRu_2S)Cl]\cdot C_2H_4Cl_2$	2.81	3.577	136.2	[2]
$[(NBu_4)(C_{11}H_9BF_2N_2O_2)Cl]\cdot ½C_2H_4Cl_2$	2.70	3.682	169.7	[3]
$[(C_6H_{12}Cl_3N_4S)Cl]\cdot C_2H_4Cl_2$	2.59	3.506	152.8	[4]
$[(C_{44}H_{52}N_4)Cl_2]\cdot 4C_2H_4Cl_2$	2.74	3.531	139.2	[5]
$[(C_{59}H_{48}OsCl_2P_3)Cl]\cdot 2C_2H_4Cl_2\cdot 2H_2O$	2.90	3.596	128.1	[6]
	2.77	3.406	122.9	
$[(C_{91}H_{77}RuClP_6)Cl_2]\cdot 2C_2H_4Cl_2\cdot 3H_2O$	2.72	3.658	162.0	[7]
$[(C_{56}H_{58}PtP_6)Cl_2]\cdot C_2H_4Cl_2$	2.67	3.412	133.7	[8]
$[(C_6HCl_9N_{10}P_3)Cl]\cdot C_2H_4Cl_2$	2.70	3.471	135.2	[9]

1. C. Zhu, M. Luo, Q. Zhu, J. Zhu, P. v. R. Schleyer, J. I.-C. Wu, X. Lu, and H. Xia, *Nat Commun*, 2014, **5**.

2. Y. Miyake, T. Moriyama, Y. Tanabe, S. Endo, and Y. Nishibayashi, *Organometallics*, 2012, **31**, 3292–3299.

3. H. Maeda and Y. Kusunose, *Chem. – A Eur. J.*, 2005, **11**, 5661–5666.

4. T. Chivers, J. F. Richardson, and N. R. M. Smith, *Inorg. Chem.*, 1985, **24**, 2453–2458.

5. D. P. Allen, C. M. Crudden, L. A. Calhoun, and R. Wang, *J. Organomet. Chem.*, 2004, **689**, 3203–3209.

6. Q. Zhao, J. Zhu, Z.-A. Huang, X.-Y. Cao, and H. Xia, *Chem. – A Eur. J.*, 2012, **18**, 11597–11603.

7. H. Zhang, R. Lin, G. Hong, T. Wang, T. Bin Wen, and H. Xia, *Chem. – A Eur. J.*, 2010, **16**, 6999–7007.

8. T. Mizuta, K. Nakayama, S. Aoki, and K. Miyoshi, *Bull. Chem. Soc. Jpn.*, 2002, **75**, 1547–1552.

9. T. Saplinova, C. Lehnert, U. Bohme, J. Wagler, and E. Kroke, *New J. Chem.*, 2010, **34**, 1893–1908.