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Supporting Information

Matrix-Isolation and Comparative Far-IR Investigation of Free Linear $[Cl_3]^-$ and the Series of the Alkaline Metal Trichlorides

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1. Experimental Details

Alkaline metal chloride targets were prepared in a hydraulic lab press and mounted on a target holder. Commercial chlorine was dried over phosphorous pentoxide and purified by trap to trap distillation. Matrix-isolation experiments were carried out in a self-built matrix chamber with a magnetic bearing motor in a distance of 40 mm from the matrix support where the targets were mounted and rotated during laser ablation. A laser beam with a wavelength of 1064 nm, a pulse length of 5 ns, and a pulse energy of up to 50 mJ was focussed on the target using a plano-convex lens with a diameter of 25.4 mm and a focal distance of 125.0 mm. The matrix support, a gold-plated copper mirror with a hole for directing the laser beam onto the target, was held at 5 K using a helium compressor unit (Sumitomo Heavy Industries 4K@0,5W) with a cryocooler coldhead. Far-IR spectra were recorded at a resolution of 0.5 cm^{-1} on a FTIR vacuum spectrometer (Bruker Vertex 80v) equipped with a transfer optic, FIR multilayer mylar beamsplitter (680-30 cm^{-1}), and a liquid helium cooled bolometer.

2. Tables

Tab. S1 Comparison of vibrational bands of isolated free $[Cl_3]^-$, alkali trichlorides and crystalline trichloride salts. Band positions in cm^{-1}.

	Band Position	Assignment	Reference
Neon			
free $[Cl_3]^-$	252	ν_{as}	This work
$Cs^+[Cl_3]^-$	218	$\nu_{Cl\text{-}ClCl}$	This work
	339	ν_{ClCl}	This work
$Rb^+[Cl_3]^-$	223	$\nu_{Cl\text{-}ClCl}$	This work
	343	ν_{ClCl}	This work
$K^+[Cl_3]^-$	245	ν_{KCl}	This work
	352	ν_{ClCl}	This work
$NaCl\cdots Cl_2$	309	ν_{NaCl}	This work
	389	ν_{ClCl}	This work
Solid			
$[n\text{-}Pr_4N]^+[Cl_3]^-$	242 (IR)	ν_{as}	[1]
	268 (R)	ν_s	[1]
$[As(C_6H_5)_4]^+[Cl_3]^-$	253 (IR)	ν_{as}	[2,3,4]
	271 (R)	ν_s	[2,3,4]
$[(Me_2NC(Cl)N)_2SCl]^+[Cl_3]^-$	268 (IR)	ν_{as}	[3]
	269 (R)	ν_s	[3]
$[P(C_6H_5)_4]^+[Cl_3]^-$	238 (IR)	ν_{as}	[4]
	268 (R)	ν_s	[4]
$[n\text{-}Pr_4N]^+[Cl_3]^-$	272 (R)	ν_s	[5]
$[n\text{-}Bu_4N]^+[Cl_3]^-$	268 (R)	ν_s	[5]
$[Bu_4N]^+_2[(Cl_3)_2Cl_2]^{2-}$	280 (R)	ν_s	[6]

[1] J. C. Evans and G. Y.-S. Lo, *J. Chem. Phys.*, 1966, **44**, 3638–3639.

[2] M. P. Bogaard, J. Peterson and A. D. Rae, *Acta Crystallogr. B*, 1981, **37**, 1357–1359.

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

[4] M. Jansen and S. Strojek, *Z. Naturforsch., B: Chem. Sci.*, 1995, **50**, 1171–1174.

[5] R. Brückner, H. Haller, M. Ellwanger and S. Riedel, *Chem. Eur. J.*, 2012, **18**, 5741–5747.

[6] R. Brückner, H. Haller, S. Steinhauer, C. Müller and S. Riedel, *Angew. Chem. Int. Ed.,* 2015, **54**, 15579–15583.

Tab. S2 Experimental structures of trichloride anions in crystalline salts for comparison with our calculated structures from Figure 1.

Crystal	a*	b*	α*	Reference
$[As(C_6H_5)_4]^+[Cl_3]^-$	222.7	230.5	177.5	[2]
$[(Me_2N)_2C_2N_4S_2Cl]^+[Cl_3]^-$	218.3	239.3	177.7	[7]
$[(Me_2NC(Cl)N)_2SCl]^+[Cl_3]^-$	224.9	234.0	177.5	[3]
$[P(C_6H_5)_4]^+[Cl_3]^-$	226.3	230.7	178.4	[4]
$[Et_4N]^+{}_2[(Cl_3)_2Cl_2]^{2-}$	223.2	234.6	176.5	[6]

* For explanations on **a**, **b** (bond lengths in pm), and α (bond angle in deg.) see Figure 1 in the main text.

[2] M. P. Bogaard, J. Peterson and A. D. Rae, *Acta Crystallogr. B*, 1981, **37**, 1357–1359.

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

[4] M. Jansen and S. Strojek, *Z. Naturforsch., B: Chem. Sci.*, 1995, **50**, 1171–1174.

[6] R. Brückner, H. Haller, S. Steinhauer, C. Müller and S. Riedel, *Angew. Chem. Int. Ed.*, 2015, **54**, 15579–15583.

[7] R. T. Boeré, A. W. Cordes, R. T. Oakley and R. W. Reed, *J. Chem. Soc. Chem. Commun.*, 1985, 655–656.

3. Figures

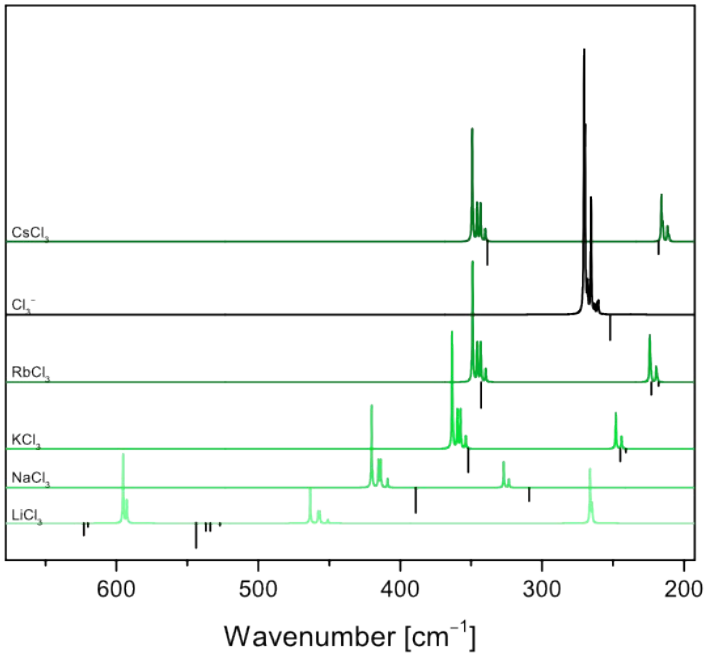

Fig. S1 Calculated (CCSD(T)/def2-TZVPP) isotope patterns of vibrations of MCl_3 and $[Cl_3]^-$ in the region from 193 to 680 cm^{-1} and comparison with experimentally observed band positions as marked by black bars pointing downwards.

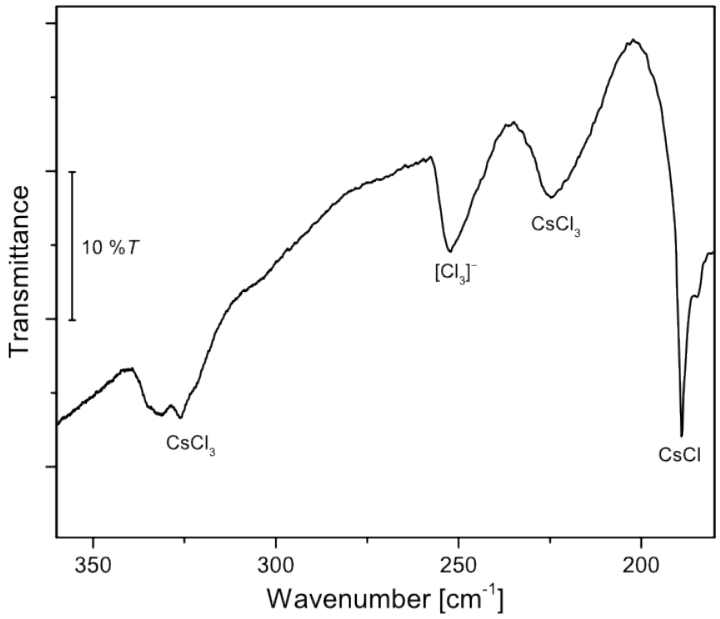

Fig. S2 FIR Spectrum measured after codeposition of laser ablated CsCl with chlorine (1 %) in solid argon at 5 K.

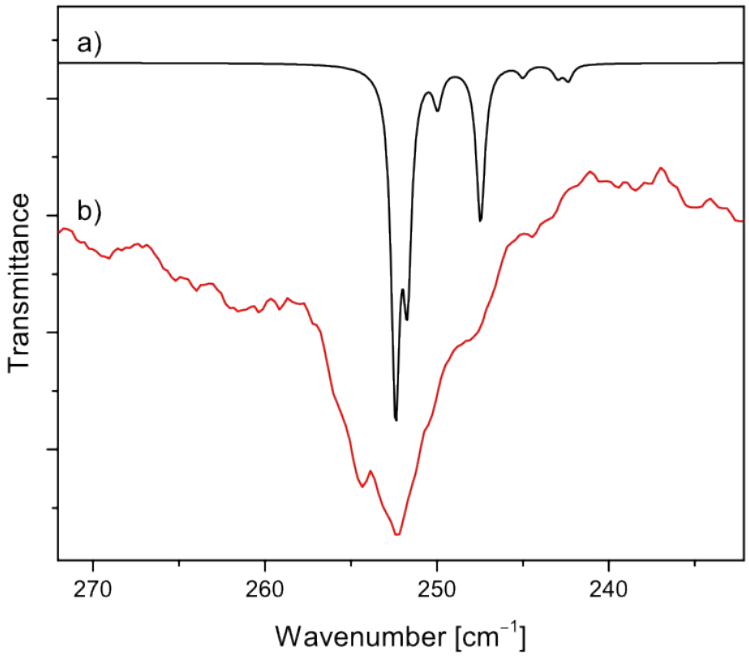

Fig. S3 Calculated (CCSD(T)/def2-TZVPP) isotope pattern of the antisymmetric stretch of $[Cl_3]^-$ with an offset of −18 cm^{-1} (a) and FIR spectrum in the region from 232 to 272 cm^{-1} obtained after codeposition of laser ablated CsCl with chlorine (0.1 %) in solid neon at 5 K showing the shape of the broad $[Cl_3]^-$ band at 252 cm^{-1} (b).

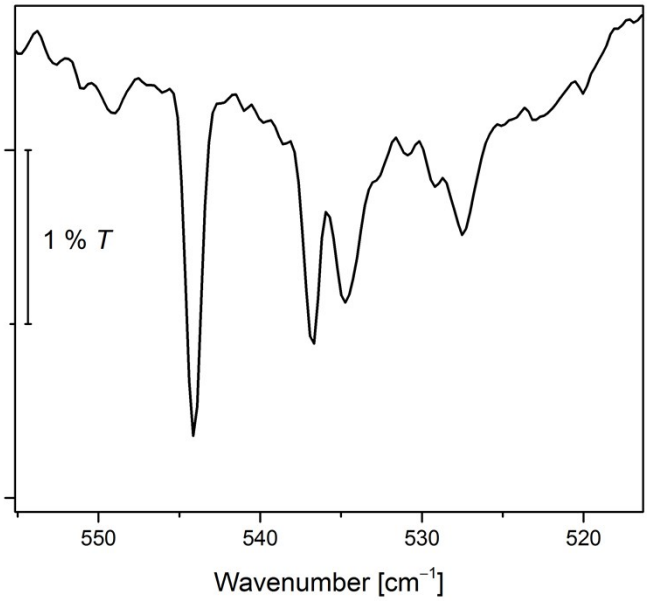

Fig. S4 IR spectrum between 515 and 555 cm^{-1} after codeposition of laser ablated LiCl with chlorine (0.1 %) in neon with pure laser ablated LiCl in neon as background.

4. Quantum Chemical Calculations

LiCl3						LiCl						Cl_2					
B3LYP/def2-TZVPP		SCS-MP2/def2-TZVPP		CCSD(T)/def2-TZVPP		B3LYP/def2-TZVPP		SCS-MP2/def2-TZVPP		CCSD(T)/def2-TZVPP		B3LYP/def2-TZVPP		SCS-MP2/def2-TZVPP		CCSD(T)/def2-TZVPP	
vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int
118	44	72	66	77	70	651	120	649	126	650	125	537	0	560	0	542	0
123	6	102	10	103	10												
145	37	115	3	117	3												
331	56	256	95	267	91												
385	176	486	57	460	69												
559	109	600	110	597	107												
E (Eh)	-	E (Eh)	-	E (Eh)	-	E (Eh)	-	E (Eh)	-	E (Eh)	-	E (Eh)	-	E (Eh)	-	E (Eh)	-
	1388.064969		1387.100255		1386.727472		467.7567837		467.4279405		467.3026344		920.2910403		919.6617193		919.4137606
ZPE (Eh)	0.00378	ZPE (Eh)	0.00371	ZPE (Eh)	0.00369	ZPE (Eh)	0.00148	ZPE (Eh)	0.00148	ZPE (Eh)	0.00148	ZPE (Eh)	0.00122	ZPE (Eh)	0.00128	ZPE (Eh)	0.00124
	-1388.06119		-1387.09654		-1386.72378		-467.75530		-467.42646		-467.30115		-920.28982		-919.66044		-919.41253
E (kJ/mol)	-	E (kJ/mol)	-3641138.17	E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-
	3643670.545				3640159.614		1227861.557		1226998.344		1226669.415		2415763.981		2414112.013		2413461.122
ZPE	9.93213375	ZPE	9.75116625	ZPE	9.69885	ZPE	3.89269125	ZPE	3.88059	ZPE	3.88644375	ZPE	3.21006	ZPE	3.35181	ZPE	3.24282
(kJ/mol)		(kJ/mol)		(kJ/mol)		(kJ/mol)		(kJ/mol)		(kJ/mol)		(kJ/mol)		(kJ/mol)		(kJ/mol)	
	-		-		-		-		-		-		-		-		-
	3643660.613		3641128.418		3640149.915		1227857.664		1226994.463		1226665.529		2415760.771		2414108.661		2413457.879
Formation:	-42	Formation:	-25	Formation:	-27												
R1	272	R1	291	R1	289	R	202	R	203	R	203	R	201	R	200	R	201
R2	212	R2	203	R2	205												
R3	210	R3	207	R3	207												
A1	170	A1	168	A1	168												
A2	55	A2	55	A2	55												
D	0	D	0	D	0												
ZMAT																	
Cl																	
Cl	1	R1															
Cl	1	R2	2	A1													
Li	2	R3	1	A2	3	D											
T1 Diagnostic for CCSD(T):				0.010523555						0.005148098						0.008340457	

NaCl3						NaCl						Cl_2					
B3LYP/def2-TZVPP		SCS-MP2/def2-TZVPP		CCSD(T)/def2-TZVPP		B3LYP/def2-TZVPP		SCS-MP2/def2-TZVPP		CCSD(T)/def2-TZVPP		B3LYP/def2-TZVPP		SCS-MP2/def2-TZVPP		CCSD(T)/def2-TZVPP	
vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int
90	10	80	4	82	6	359	44	362	51	364	50	537	0	560	0	542	0
131	1	101	112	108	109												
147	83	122	2	121	2												
201	18	173	24	176	25												
307	32	329	43	326	39												
370	221	437	154	417	162												
E (Eh)	-	E (Eh)	-	E (Eh)	-	E (Eh)	-	E (Eh)	-	E (Eh)	-	E (Eh)	-	E (Eh)	-	E (Eh)	-
	1542.807435		1541.620026		1541.260963		622.4974559		621.9460427		621.8343698		920.2910403		919.6617193		919.4137606
ZPE (Eh)	0.00284	ZPE (Eh)	0.00283	ZPE (Eh)	0.00280	ZPE (Eh)	0.00082	ZPE (Eh)	0.00083	ZPE (Eh)	0.00083	ZPE (Eh)	0.00122	ZPE (Eh)	0.00128	ZPE (Eh)	0.00124
	-1542.80459		-1541.61720		-1541.25816		-622.49664		-621.94522		-621.83354		-920.28982		-919.66044		-919.41253
E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-
	4049869.516		4046752.567		4045810.027		1634055.822		1632608.362		1632315.221		2415763.981		2414112.013		2413461.122
ZPE	7.45563	ZPE	7.4202975	ZPE	7.35546	ZPE	2.14900875	ZPE	2.16680625	ZPE	2.17494375	ZPE	3.21006	ZPE	3.35181	ZPE	3.24282
(kJ/mol)		(kJ/mol)		(kJ/mol)		(kJ/mol)		(kJ/mol)		(kJ/mol)		(kJ/mol)		(kJ/mol)		(kJ/mol)	
	-4049862.06		-		-		-		-		-		-		-		-
			4046745.147		4045802.672		1634053.673		1632606.195		1632313.046		2415760.771		2414108.661		2413457.879
Formation:	-48	Formation:	-30	Formation:	-32												
R1	264	R1	276	R1	275	R	236	R	236	R	236	R	201	R	200	R	201
R2	215	R2	206	R2	208												
R3	246	R3	242	R3	242												
A1	174	A1	174	A1	173												
A2	63	A2	64	A2	64												
D	0	D	0	D	0												
ZMAT																	
Cl																	
Cl	1 R1																
Cl	1 R2	2 A1															
Na	2 R3	1 A2		3 D													
T1 Diagnostic for CCSD(T):				0.011077804						0.006674233						0.008340457	

KCl3						KCl						Cl_2					
B3LYP/def2-TZVPP		SCS-MP2/def2-TZVPP		CCSD(T)/def2-TZVPP		B3LYP/def2-TZVPP		SCS-MP2/def2-TZVPP		CCSD(T)/def2-TZVPP		B3LYP/def2-TZVPP		SCS-MP2/def2-TZVPP		CCSD(T)/def2-TZVPP	
vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int
65	3	64	2	65	1	272	50	276	53	276	52	537	0	560	0	542	0
141	1	136	202	139	164												
157	84	146	1	140	5												
196	15	194	15	190	17												
235	45	249	68	247	58												
343	238	361	250	361	242												
E (Eh)	-	E (Eh)	-	E (Eh)	-	E (Eh)	-	E (Eh)	-	E (Eh)	-	E (Eh)	-	E (Eh)	-	E (Eh)	-
	1980.419029		1978.927228		1978.570083		1060.105436		1059.250013		1059.140363		920.2910403		919.6617193		919.4137606
ZPE (Eh)	0.00259	ZPE (Eh)	0.00262	ZPE (Eh)	0.00260	ZPE (Eh)	0.00062	ZPE (Eh)	0.00063	ZPE (Eh)	0.00063	ZPE (Eh)	0.00122	ZPE (Eh)	0.00128	ZPE (Eh)	0.00124
	-1980.41644		-1978.92461		-1978.56748		-1060.10482		-1059.24938		-1059.13973		-920.28982		-919.66044		-919.41253
E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-
	5198599.952		5194683.975		5193746.467		2782776.768		2780531.284		2780243.453		2415763.981		2414112.013		2413461.122
ZPE	6.80266125	ZPE	6.874455	ZPE	6.83101125	ZPE	1.62379875	ZPE	1.64871	ZPE	1.6512825	ZPE	3.21006	ZPE	3.35181	ZPE	3.24282
(kJ/mol)		(kJ/mol)		(kJ/mol)		(kJ/mol)		(kJ/mol)		(kJ/mol)		(kJ/mol)		(kJ/mol)		(kJ/mol)	
	-		-5194677.1		-		-		-		-		-		-		-
	5198593.149				5193739.636		2782775.144		2780529.635		2780241.802		2415760.771		2414108.661		2413457.879
Formation:	-57	Formation:	-39	Formation:	-40												
R1	256	R1	256	R1	259	R	270	R	271	R	271	R	201	R	200	R	201
R2	218	R2	212	R2	213												
R3	285	R3	282	R3	282												
A1	173	A1	174	A1	174												
A2	66	A2	68	A2	67												
D	0	D	0	D	0												
ZMAT																	
Cl																	
Cl	1	R1															
Cl	1	R2	2	A1													
K	2	R3	1	A2	3	D											
T1 Diagnostic for CCSD(T):				0.011897693					0.00544501								0.008340457

$RbCl_3$						$RbCl$						Cl_2					
B3LYP/def2-TZVPP		SCS-MP2/def2-TZVPP		CCSD(T)/def2-TZVPP		B3LYP/def2-TZVPP		SCS-MP2/def2-TZVPP		CCSD(T)/def2-TZVPP		B3LYP/def2-TZVPP		SCS-MP2/def2-TZVPP		CCSD(T)/def2-TZVPP	
vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int
50	2	48	2	50	1	222	41	227	45	228	45	537	0	560	0	542	0
137	62	135	157	136	140												
142	1	152	1	144	1												
181	6	184	25	179	14												
218	69	227	122	223	96												
334	240	341	258	347	253												
E (Eh)	-	E (Eh)	-	E (Eh)	-	E (Eh)	-	E (Eh)	-	E (Eh)	-	E (Eh)	-	E (Eh)	-	E (Eh)	-
	1404.632055		1403.511566		1403.153112		484.3176997		483.8333649		483.7223923		920.2910403		919.6617193		919.4137606
ZPE (Eh)	0.00242	ZPE (Eh)	0.00248	ZPE (Eh)	0.00246	ZPE (Eh)	0.00051	ZPE (Eh)	0.00052	ZPE (Eh)	0.00052	ZPE (Eh)	0.00122	ZPE (Eh)	0.00128	ZPE (Eh)	0.00124
	-1404.62963		-1403.50909		-1403.15065		-484.31719		-483.83285		-483.72187		-920.28982		-919.66044		-919.41253
E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-1269771.28	E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-
	3687159.144		3684217.861		3683276.918		1271333.962		1270062.583				2415763.981		2414112.013		2413461.122
ZPE	6.35273625	ZPE	6.5028075	ZPE	6.45211875	ZPE	1.33042875	ZPE	1.3573875	ZPE	1.36497375	ZPE	3.21006	ZPE	3.35181	ZPE	3.24282
(kJ/mol)		(kJ/mol)		(kJ/mol)		(kJ/mol)		(kJ/mol)		(kJ/mol)		(kJ/mol)		(kJ/mol)		(kJ/mol)	
	-		-		-		-		-		-		-		-		-
	3687152.792		3684211.358		3683270.466		1271332.631		1270061.225		1269769.915		2415760.771		2414108.661		2413457.879
Formation:	-59	Formation:	-41	Formation:	-43												
R1	253	R1	251	R1	255	R	286	R	286	R	285	R	201	R	200	R	201
R2	220	R2	214	R2	214												
R3	303	R3	299	R3	298												
A1	173	A1	174	A1	174												
A2	68	A2	69	A2	68												
D	0	D	0	D	0												
ZMAT																	
Cl																	
Cl	1 R1																
Cl	1 R2	2 A1															
Rb	2 R3	1 A2	3 D														
T1 Diagnostic for CCSD(T):			0.012569785						0.007092337						0.008340457		

$CsCl_3$						CsCl						Cl_2					
B3LYP/def2-TZVPP		SCS-MP2/def2-TZVPP		CCSD(T)/def2-TZVPP		B3LYP/def2-TZVPP		SCS-MP2/def2-TZVPP		CCSD(T)/def2-TZVPP		B3LYP/def2-TZVPP		SCS-MP2/def2-TZVPP		CCSD(T)/def2-TZVPP	
vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int
41	1	37	3	40	1	209	54	205	58	205	58	537	0	560	0	542	0
125	55	122	122	123	113												
142	1	152	1	145	1												
178	11	176	51	170	33												
214	71	221	124	215	100												
333	231	341	246	347	241												
E (Eh)	-	E (Eh)	-	E (Eh)	-	E (Eh)	-	E (Eh)	-	E (Eh)	-	E (Eh)	-	E (Eh)	-	E (Eh)	-
	1400.690059		1399.612316		1399.260367		480.3772594		479.9345621		479.8302693		920.2910403		919.6617193		919.4137606
ZPE (Eh)	0.00235	ZPE (Eh)	0.00239	ZPE (Eh)	0.00237	ZPE (Eh)	0.00048	ZPE (Eh)	0.00047	ZPE (Eh)	0.00047	ZPE (Eh)	0.00122	ZPE (Eh)	0.00128	ZPE (Eh)	0.00124
	-1400.68771		-1399.60993		-1399.25800		-480.37678		-479.93409		-479.82980		-920.28982		-919.66044		-919.41253
E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-
	3676811.405		3673982.329		3673058.464		1260990.306		1259828.226		1259554.457		2415763.981		2414112.013		2413461.122
ZPE	6.1764675	ZPE	6.27188625	ZPE	6.2118	ZPE	1.2480825	ZPE	1.22661	ZPE	1.22787	ZPE	3.21006	ZPE	3.35181	ZPE	3.24282
(kJ/mol)		(kJ/mol)		(kJ/mol)		(kJ/mol)		(kJ/mol)		(kJ/mol)		(kJ/mol)		(kJ/mol)		(kJ/mol)	
	-		-		-		-		-		-		-		-		-
	3676805.229		3673976.057		3673052.252		1260989.058		1259826.999		1259553.229		2415760.771		2414108.661		2413457.879
Formation:	-55	Formation:	-40	Formation:	-41												
R1	253	R1	251	R1	255	R	295	R	295	R	295	R	201	R	200	R	201
R2	220	R2	214	R2	214												
R3	315	R3	312	R3	311												
A1	173	A1	174	A1	174												
A2	69	A2	70	A2	70												
D	0	D	0	D	0												
ZMAT																	
Cl																	
Cl	1 R1																
Cl	1 R2	2 A1															
Cs	2 R3	1 A2		3 D													
T1 Diagnostic for CCSD(T):				0.012210276						0.005758204						0.008340457	

$[Cl_3]^-$						Cl^-						Cl_2					
B3LYP/def2-TZVPP		SCS-MP2/def2-TZVPP		CCSD(T)/def2-TZVPP		B3LYP/def2-TZVPP		SCS-MP2/def2-TZVPP		CCSD(T)/def2-TZVPP		B3LYP/def2-TZVPP		SCS-MP2/def2-TZVPP		CCSD(T)/def2-TZVPP	
vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int	vib/cm^{-1}	Int
154	2	168	1	163	2							537	0	560	0	542	0
246	0	271	0	263	0												
258	409	293	578	269	614												
			-		-		-		-		-	E (Eh)	-	E (Eh)	-	E (Eh)	-
E (Eh)	-1380.5651	E (Eh)	1379.60625	E (Eh)	1379.23415	E (Eh)	460.220098	E (Eh)	459.901907	E (Eh)	459.777708		920.2910403		919.6617193		919.4137606
ZPE (Eh)	0.00185	ZPE (Eh)	0.00205	ZPE (Eh)	0.00195							ZPE (Eh)	0.00122	ZPE (Eh)	0.00128	ZPE (Eh)	0.00124
	-		-		-								-920.28982		-919.66044		-919.41253
	1380.56325		1379.60420		1379.23220		-460.22010		-459.90191		-459.77771						
					-		-		-		-	E (kJ/mol)	-	E (kJ/mol)	-	E (kJ/mol)	-
E (kJ/mol)	-3623983.4	E (kJ/mol)	-3621466.4	E (kJ/mol)	3620489.65	E (kJ/mol)	1208077.76	E (kJ/mol)	1207242.51	E (kJ/mol)	1206916.48		2415763.981		2414112.013		2413461.122
ZPE		ZPE		ZPE		ZPE		ZPE		ZPE		ZPE	3.21006	ZPE	3.35181	ZPE	3.24282
(kJ/mol)	4.85391375	(kJ/mol)	5.37705	(kJ/mol)	5.1300375	(kJ/mol)	0	(kJ/mol)	0	(kJ/mol)	0	(kJ/mol)		(kJ/mol)		(kJ/mol)	
	-		-		-		-		-		-		-		-		-
	3623978.54		3621461.02		3620484.52		1208077.76		1207242.51		1206916.48		2415760.771		2414108.661		2413457.879
Formation:	-140	Formation:	-110	Formation:	-110												
R1	235	R1	231	R1	232							R	201	R	200	R	201
R2	235	R2	231	R2	232												
A	180	A	180	A	180												
ZMAT																	
Cl																	
Cl	1 R1																
Cl	1 R2	2 A															
T1 Diagnostic for CCSD(T):				0.01421577						0.003500188						0.008340457	