SUPPLEMENTARY MATERIAL

Table S1. Triplet-singlet energy splitting (in kcal mol^{-1}) of HCCl (DCCl).

	Authors and year	Ref.	Method[a]	Comment
Experimental				
11±0.3	Lineberger et al. 1988	21	PDS	b
4.2±2.5	Lineberger et al. 1992	22	PDS	b
8 (11±2)	Chang et al. 2001 (2002)	13,14	LIDF	c
6.20±0.025 (6.25±0.05)	Chang et al. 2004	17	LIDF	c
Calculated				
1.6	Bauschlicher et al. 1977	56	GVB(1/2)	e
5.4	Schaefer et al. 1986	57	TCSCF	e
5.8	Goddard et al. 1987	58,59	GVB-RCI	e
6.7	Goddard et al. 1987	58,59	GVB-RCI	e
5.6±0.7	Goddard et al. 1987	58,59	FCI	e
9.3	Goddard et al. 1987	58,59	GVB-CCCI	e
6.0	Goddard et al. 1990	60	GVB-DCCI	e
6.4±0.7	Goddard et al. 1990	60	GVB-DCCI	e
6.39	Goddard et al. 1992	61	GVB(1/2)	e
4.8	Gobbi and Frenking 1993	62	MP4	d, f
5.8	Caballol et al. 1996	63	DDCI	d, h
6.2	Worthington and Cramer 1997	64	DFT	d
9.0	Schwartz and Marshall 1999	65	G2	d
5.7	Schwartz and Marshall 1999	65	QCISD(T)	d
0.9−2.4	Hajgató et al. 2000	66	CASPT2	d, f, h
4.8−6.6	Hajgató et al. 2000	66	CCSD(T)	d, f, h
6.1	Bacskay et al. 2000	67	MRCI+D	d, h
6.6	Bacskay et al. 2000	67	CCSD(T)	d, h
6.1	Radom et al. 2001	68	DFT (BLYP)	d
6.8	Radom et al. 2001	68	G3(MP2)	d, f
5.9	Radom et al. 2001	68	W1'	d
6.204±0.114 (6.207±0.114)	This study 2005		FPA	d, f, g

[a] PDS: Photodetachment Spectroscopy, LIDF: Laser-Induced Dispersed Fluorescence, GVB: Generalized Valence Bond Theory, TCSCF: Two-Configuration Self Consistent Field, GVB-RCI: GVB-Restricted Configuration Interaction, FCI: Full Configuration Interaction, GVB-CCCI: GVB-Correlation-Consistent configuration interaction method, GVB-DCCI: GVB-Dissociation Consistent Configuration Interaction, MP4: 4th-order Møller−Plesset Perturbation Theory, DDCI: Difference Dedicated Configuration Interaction, DFT:

Density Functional Theory, G2: Gaussian 2 Theory, QCISD(T): Quadratic Configuration Interaction with Singles, Doubles and Perturbative Triples, CASPT2: Complete Active Space (2nd-order) Perturbation Theory, CCSD(T): Coupled Cluster Theory with Singles Doubles and Perturbative Triples, MRCI+D: Multi-Reference Configuration Interaction with Davidson Correction, BLYP: Becke Exchange + LYP (Lee-Yang-Parr) Correlation Functional, G3(MP2): Modified Gaussian 3 Theory, W1': Modified Weizmann 1 Theory, FPA: Focal-Point Approach.

[b] ΔE_{TS} is obtained by Franck−Condon envelope simulation of the spectrum.

[c] Ref. 17 reports reassigned, higher resolution and lower signal-to-noise data as compared to refs. 13 and 14.

[d] ΔE_{TS} corrected for zero-point vibrational energy, i.e. $T_0\left(\tilde{a}\right)$.

[e] ΔE_{TS} not corrected for zero-point vibrational energy, i.e. $T_{\mathrm{e}}\left(\tilde{a}\right)$.

[f] Relativistic correction included.

[g] Diagonal Born−Oppenheimer Correction (DBOC) included.

[h] Paper reports further results obtained at lower level of theory.

Table S2. Enthalpies of formation ($\Delta_f H^{o}_{298}$ in kcal mol^{-1}) of $\tilde{X}\,^1A'$ HCCl.

	Authors and year	Ref.	Method[a]	Comment
Experimental				
71±5	Lias et al. 1985	45	ICR	b
75.7±4.8	Born et al. 1994	46	ICR	c
80.4±2.8	Poutsma et al. 1997	47	CID	d
Calculated				
77.4	Rodriquez et al. 1996	82	MP4	e
76.8	Rodriquez et al. 1996	82	QCISD(T)	e
75.4	Poutsma et al. 1997	47	G2	e
76.0	Poutsma et al. 1997	47	G2	f
76.1	Schwartz and Marshall 1999	65	G2	f
76.4	Schwartz and Marshall 1999	65	QCISD(T)	f
75.3	Sendt and Bacskay 2000	77	G2	e
76.1	Sendt and Bacskay 2000	77	G3	e
76.5±1	Sendt and Bacskay 2000	77	CCSD(T)	e, g
76.35±0.20	This study 2005		FPA	h
Reviews and evaluations				
80±10	JANAF (Stull and Prophet) 1971	143		
80±10	JANAF (Chase et al.) 1985, 1998	144		
71	Lias et al. 1988	145		
73.6±7	Gurvich et al. 1992	146		
78.0±2.0	Poutsma et al. 1997	47		i

[a] ICR: Ion Cyclotron Resonance, CID: Collision Induced Dynamics, MP4: 4th-order Møller−Plesset Perturbation Theory QCISD(T): Quadratic Configuration Interaction with Singles, Doubles and Perturbative Triples, G2: Gaussian 2 Theory, G3: Gaussian 3 Theory, FPA: Focal-Point Approach.

[b] Bracketing the proton affinity of CCl_2H^+ by B: + CCl_2H^+ → BH^+ + CCl_2 processes, where B: various bases.

[c] Determined from the heat of the $HCCl^- + HA \rightarrow H_2CCl + A^-$ reaction, where HA: CH_3Cl, CH_3OH.

[d] Obtained from the threshold energy of the $CH_2Cl^- \rightarrow HCCl + Cl^-$ dissociation reaction.

[e] Determined from the calculated atomization energies and the measured heats of formations of the corresponding atoms.

[f] Determined from the calculated enthalpy change of the $HCCl + CH_4 \rightarrow CH_3Cl + CH_2(^1A_1)$ reaction and experimental heats of formations of CH_4, CH_3Cl, and $CH_2(^1A_1)$.

[g] Complete basis set extrapolated CCSD(T) energy + relativistic correction.

[h] Determined from the calculated enthalpy change of the $CH_2(\tilde{a}\,^1A_1) + HCl(\tilde{X}\,^1\Sigma^+) \rightarrow HCCl(\tilde{X}\,^1A') + H_2(\tilde{X}\,^1\Sigma_g)$ reaction and experimental enthalpies of formation of HCl, H_2, and $CH_2(^1A_1)$.

[i] Evaluated from G2 calculation and experimental results.

Table S3. Triplet-singlet energy splitting (in kcal mol^{-1}) of CCl_2.

	Authors and year	Ref.	Method[a]	Comment
Experimental				
3±3	Lineberger et al. 1999	42	PDS	b
>17	Liu et al. 2003	43	LIDF	c
Calculated				
13.5	Bauschlicher et al. 1977	56	GVB(1/2)	e
19.1	Ha et al. 1979	70	CISD	e
21.9	Nguyen et al. 1985	71	MP4SDQ	e, h
21.1	Goddard et al. 1987	58,59	GVB-RCI	e
23.2	Goddard et al. 1987	58,59	GVB-RCI	e
21.6±1.4	Goddard et al. 1987	58,59	FCI	e
25.9	Goddard et al. 1987	58,59	GVB-CCCI	e
20.5±1	Goddard et al. 1990	60	GVB-DCCI	e
23.7	Ziegler et al. 1991	72	DFT	e, f
20.0	Goddard et al. 1992	61	GVB(1/2)	e
23.7	Russo et al. 1992	73	DFT (LCGTO−LSD)	d
20.5	Gobbi and Frenking 1993	62	MP4	d, f
19.7	Caballol et al. 1996	63	DDCI	d, h
21.0	Das and Whittenburg 1999	74	DFT (B3LYP)	d
23.1	Schwartz and Marshall 1999	65	G2	d
19.6	Schwartz and Marshall 1999	65	QCISD(T)	d
19.5±2	Barden and Schaefer 2000	75	CCSD(T)	e, h
20.0±1	Wright et al. 2000	76	CCSD(T), MRCI+D	e, h
19.2	Sendt and Bacskay 2000	77	MRCI+D	d, h
20.9	Sendt and Bacskay 2000	77	CCSD(T)	d, h
14.7−17.8	Hajgató et al. 2000	66	CASPT2	d, f, h
18.4−21.5	Hajgató et al. 2000	66	CCSD(T)	d, f, h
21.0	Radom et al. 2001	68	DFT (BLYP)	d
21.5	Radom et al. 2001	68	G3(MP2)//B3LYP	d, f
19.9	Radom et al. 2001	68	W1'	d
19.8	Szabados and Hargittai 2003	80	CCSD(T)	e
20.13±0.17	This study 2005		FPA	d, f, g

[a] CISD: Configuration Interaction with Single and Double Excitations, MP4SDQ: 4th-order Møller−Plesset Perturbation Theory with Single, Double and Quadruple Excitations, LCGTO-LSD: Linear Combination of Gaussian-type Orbitals-Local Spin Density Method. See footnote a to Table S1 for other abbreviations.

[b] Alternative interpretation of the PD spectrum is available. See text for details.

[c] Low limit. See text for details.

[d] ΔE_{TS} corrected for zero-point vibrational energy, i.e. $T_0\left(\tilde{a}\right)$.

[e] ΔE_{TS} not corrected for zero-point vibrational energy, i.e. $T_{\mathrm{e}}\left(\tilde{a}\right)$.

[f] Relativistic correction is included.

[g] Diagonal Born−Oppenheimer Correction (DBOC) included.

[h] Paper reports further results obtained at lower level of theory.

Table S4. Enthalpies of Formation ($\Delta_f H^{o}_{298}$ in kcal mol^{-1}) of $\tilde{X}\,^1A_1$ CCl$_2$.

	Authors and year	Ref.	Method[a]	Comment
Experimental				
47±3	Benson and Spokes 1967	48	KIN	b
56.5±5	Saphiro and Lossing 1968	49	EI	c
44±2	Lias and Ausloos 1976	50	ICR	d
53.8±2	Levi et al. 1977	51	ICR	e
47.8±2	Ausloos and Lias 1978	52	ICR	d
37±7	Verhaart et al. 1980	53	EI	f
39±3	Lias et al. 1985	45	ICR	d
52.1±3.4	Paulino and Squires 1991	54	CID	g
51.0±2.0	Kohn et al. 1993	55	PES	h
55.0±2.0	Poutsma et al. 1997	47	CID	g
Calculated				
55.3	Rodriquez et al. 1996	82	MP4	i
54.5	Rodriquez et al. 1996	82	QCISD(T)	i
53.5	Poutsma et al. 1997	47	G2	i
53.7	Poutsma et al. 1997	47	G2	j
53.49	Cheong et al. 1997	83	G2	i
51.13	Cheong et al. 1997	83	G2(MP2)	i
52.23	Cheong et al. 1997	83	CBS-Q	i
53.14	Cheong et al. 1997	83	CBS-4	i
54.3	Schwartz and Marshall 1999	65	G2	i
55.0	Schwartz and Marshall 1999	65	QCISD(T)	i
53.4	Sendt and Bacskay 2000	77	G2	i
54.3	Sendt and Bacskay 2000	77	G3	i
54.7±1	Sendt and Bacskay 2000	77	CCSD(T)	i, k, l
55.4±0.4	Dixon and Peterson 2001	78	CCSD(T)	i, k, l
54.8±0.4	Demaison et al. 2002	79	W2	i
54.83±0.20	This study 2005		FPA	m
Reviews and evaluations				
57±5	JANAF (Stull and Prophet) 1971	143		
57±5	JANAF (Chase et al.) 1985	144		
39	Lias et al. 1988	145		
54±5	Gurvich et al. 1992	146		
57.2±4.0	Grabowski et al. 1992	147		
55.0±2.0	Kerr and Stocker 2000	148		

[a] KIN: Kinetic Study, EI: Electron Impact Measurements, PES: Photoelectron Spectroscopy, G2(MP2): Modified G2 Theory, CBS(-Q and -4): (Different Versions of) Complete Basis Set Model Chemistry, W2: Weizmann 2 Theory. See also footnote a of Table S2.

[b] Determined from kinetic studies of processes, e.g. $CHCl_3 \leftrightarrow HCl + CCl_2$.

[c] Determined from the energetics of the $CHCl_3 + e^- \rightarrow CCl_2^+ + HCl + 2e^-$ and the $C_2Cl_4 + e^- \rightarrow CCl_2^+ + CCl_2 + 2e^-$ processes and ionization potential of CCl_2.

[d] Bracketing the proton affinity of CCl_2H^+ by $B: + CCl_2H^+ \rightarrow BH^+ + CCl_2$ processes, where B: various bases.

[e] Obtained from the measurement of the enthalpy of the $B: + CCl_2H^+ \rightarrow BH^+ + CCl_2$ process, where B: is $CF_3CH_2CH_2NH_2$, 2-triflouromethyl-pyridine.

[f] Determined from the energy threshold of the $CH_4 + e^- \rightarrow CCl_2 + Cl_2^-$ process.

[g] Obtained from the threshold energy of the $CCl_3^- \rightarrow CCl_2 + Cl^-$ dissociation process.

[h] Obtained from accurate ionization potential measurement of CCl_2 and using former $\Delta_f H^{o}_{298}$ value for CCl_2^+.

[i] Determined from the calculated atomization energies and the measured heats of formations of the corresponding atoms.

[j] Determined from the calculated enthalpy change of the $CCl_2 + 2\ CH_4 \rightarrow 2\ CH_3Cl + CH_2(^1A_1)$ reaction and experimental enthalpies of formations of CH_4, CH_3Cl, and $CH_2(^1A_1)$.

[k] Complete basis set extrapolated CCSD(T) energy + relativistic correction.

[l] Reference gave $\Delta_f H^{o}_{0}$ only. $\Delta_f H^{o}_{298}$ was obtained as $\Delta_f H^{o}_{0}$ + 0.29 kcal mol^{-1}. See text for details.

[m] Determined from the calculated enthalpy change of the $CH_2(\tilde{a}\,^1A_1) + 2\ HCl(\tilde{X}\,^1\Sigma^+) \rightarrow CCl_2(\tilde{X}\,^1A_1) + 2\ H_2(\tilde{X}\,^1\Sigma_g)$ reaction and experimental enthalpies of formation of HCl, H_2, and $CH_2(^1A_1)$.

Table S5. Variationally calculated $\tilde{X}$ state vibrational energy levels of several isotopologs HCCl.

HC^{35}Cl		**HC^{37}Cl**	**DC^{35}Cl**		**DC^{37}Cl**
Var4	Var4^{+}	Var4	Var4	Var4^{+}	Var4
2452.5	2452.4	2449.3	1916.3	1916.3	1913.0
809.8	809.8	804.1	799.6	799.7	793.5
1199.8	1199.6	1199.3	896.1	896.0	895.6
1609.6	1609.6	1598.2	1589.9	1589.9	1577.8
2001.8	2001.6	1995.6	1691.4	1691.3	1684.8
2382.3	2381.1	2381.1	1779.2	1778.8	1778.3
2399.5	2399.5	2382.7	2076.0	2076.0	2076.0
2785.0	2785.0	2780.0	2370.7	2370.7	2352.7
2795.2	2795.0	2788.6	2477.1	2477.0	2464.6
3176.6	3175.5	3157.3	2570.3	2570.0	2563.4
3179.6	3179.6	3170.1	2651.2	2649.9	2649.9
3548.9	3545.8	3547.2	2873.6	2873.6	2867.5
3573.9	3573.8	3557.4	2973.4	2973.3	2972.8
3599.1	3599.0	3592.7	3142.1	3142.1	3118.5
3949.7	3949.8	3922.3	3253.2	3253.2	3235.0
3959.9	3959.0	3948.3	3351.7	3351.4	3338.9
3979.2	3978.7	3978.2	3438.0	3436.9	3430.8
4335.9	4332.9	4324.0	3513.4	3510.7	3511.5
4346.1	4346.1	4328.9	3662.0	3662.0	3650.0
4399.4	4399.4	4387.8	3766.2	3766.1	3759.6
4701.4	4694.9	4678.0	3852.0	3851.5	3851.0
4710.4	4710.5	4698.9	3904.2	3904.2	3875.1
4734.0	4733.2	4716.9	4019.9	4019.9	3996.1
4781.8	4781.4	4775.4	4083.6	4083.6	4083.5
5108.1	5107.7	5081.0	4123.4	4123.2	4104.9
5112.3	5109.9	5099.9	4214.9	4214.0	4201.9
5146.0	5144.2	5144.8	4295.6	4293.2	4287.9
5190.0	5190.0	5172.9	4367.0	4362.2	4364.6
5446.5	5446.5	5424.2	4441.3	4441.3	4423.5
5461.6	5461.7	5446.5	4549.7	4549.7	4537.2
5480.9	5474.6	5473.2	4641.0	4640.5	4622.5
5498.0	5497.4	5475.9	4657.1	4657.1	4634.0
5574.5	5574.2	5562.7	4716.4	4715.0	4715.0
5840.9	5829.6		4777.2	4777.2	
5860.6	5860.8		4878.2	4878.2	
5878.6	5876.0		4885.5	4885.4	
5941.8	5940.1		4982.0	4981.2	
5970.8	5970.8		4987.1	4987.0	
6203.4	6203.6		5067.7	5065.6	
6249.5	6243.6		5144.1	5139.6	

Table S6. Variationally calculated $\tilde{a}$ state vibrational energy levels of several isotopologs HCCl.

HC^{35}Cl		**HC^{37}Cl**	**DC^{35}Cl**		**DC^{37}Cl**
Var4	Var4^{+}	Var4	Var4	Var4^{+}	Var4
2499.8	2499.6	2496.4	1966.4	1966.4	1962.9
883.3	883.3	876.9	707.6	707.2	706.6
943.4	942.2	943.2	879.4	879.4	873.6
1756.4	1756.4	1743.8	1408.3	1406.3	1406.4
1825.1	1823.9	1818.4	1579.0	1578.3	1572.0
1864.4	1858.0	1863.9	1748.3	1748.2	1736.8
2619.5	2619.5	2600.7	2101.1	2095.1	2098.5
2696.2	2695.1	2683.2	2271.0	2268.2	2263.3
2742.1	2733.1	2735.7	2288.9	2288.8	2288.5
2764.0	2746.6	2762.7	2440.2	2439.1	2427.4
3071.1	3071.2	3071.1	2607.0	2606.8	2589.9
3472.4	3472.5	3447.7	2784.8	2770.3	2781.8
3556.8	3555.8	3537.8	2956.2	2948.5	2947.5
3606.9	3570.2	3595.9	2990.3	2989.9	2988.9
3625.5	3606.4	3620.1	3125.1	3121.3	3111.2
3654.3	3630.7	3649.3	3169.7	3169.7	3163.8
3950.6	3950.7	3944.4	3291.4	3289.9	3272.9
4006.3	4005.6	4005.9	3455.6	3425.9	3433.1
4315.3	4315.4	4284.7	3457.8	3455.3	3454.4
4407.1	4335.6	4382.2	3632.9	3615.2	3623.5
4448.4	4406.3		3685.0	3683.3	
4470.1	4447.7		3802.9	3793.1	
4505.3	4473.3		3862.8	3862.2	
4539.6	4507.4		3969.2	3964.2	
4820.6	4820.6		4039.6	4039.5	
4884.4	4883.5		4117.4	4050.1	
4918.7	4914.0		4132.8	4130.8	

Table S7. Variationally calculated $\tilde{X}$ state vibrational energy levels of $C^{35}Cl_2$ and $C^{35}Cl^{37}Cl$.

$C^{35}Cl_2$											**$C^{35}Cl^{37}Cl$**
Var4											Var4
920.7	2874.2	3785.4	4442.0	4968.4	5393.6	5791.2	6118.4	6430.7	6698.8	6958.1	916.3
334.9	2878.2	3814.4	4450.6	4979.0	5401.0	5795.4	6128.9	6431.3	6703.0	6968.5	330.8
669.4	2898.0	3824.6	4470.7	4982.9	5410.8	5797.4	6130.1	6432.6	6709.0	6970.4	661.1
727.3	2898.9	3849.9	4472.9	4997.4	5427.5	5806.3	6137.8	6446.2	6724.2	6984.0	724.8
759.5	2934.1	3860.1	4497.1	5010.0	5437.4	5808.8	6146.4	6447.2	6724.5	6985.3	757.6
1003.4	2970.9	3861.4	4501.3	5012.4	5444.0	5810.1	6154.5	6448.9	6727.5	6993.3	991.1
1060.6	2991.1	3873.4	4515.2	5025.6	5458.4	5828.7	6170.2	6464.6	6728.6	6995.5	1054.0
1090.0	2997.4	3901.9	4521.6	5027.3	5468.5	5830.5	6176.7	6469.4	6744.0	7001.4	1084.1
1337.1	3054.0	3904.5	4546.5	5043.2	5483.9	5838.5	6181.6	6471.4	6745.1	7011.2	1320.6
1393.7	3062.5	3918.1	4557.3	5065.5	5487.3	5852.0	6191.1	6487.3	6747.4	7011.4	1383.0
1420.1	3105.7	3933.7	4562.5	5071.1	5487.6	5857.5	6196.9	6494.5	6757.4	7022.3	1410.0
1448.8	3121.5	3946.1	4574.9	5071.6	5489.3	5857.7	6208.4	6504.6	6762.8	7024.8	1443.7
1480.9	3137.6	3954.6	4581.1	5076.2	5510.0	5876.7	6210.0	6504.8	6766.6	7032.7	1476.7
1510.7	3155.1	3986.2	4595.7	5085.4	5521.3	5879.1	6216.8	6513.9	6779.5	7035.9	1506.8
1670.2	3173.5	3987.4	4600.1	5086.1	5531.9	5898.2	6224.4	6516.9	6783.0	7038.0	1649.8
1726.5	3202.0	4026.3	4604.2	5116.8	5535.1	5899.6	6229.3	6517.0	6784.0	7038.6	1711.7
1749.6	3203.3	4038.2	4624.0	5117.1	5537.4	5899.8	6232.2	6523.3	6802.9	7045.4	1735.6
1780.6	3219.9	4040.8	4641.8	5121.2	5560.0	5901.8	6240.5	6533.5	6810.2	7047.4	1771.4
1809.8	3223.6	4044.0	4644.5	5139.7	5560.9	5913.5	6243.7	6539.1	6818.6	7055.6	1801.6
1837.1	3257.1	4093.6	4661.3	5144.7	5574.6	5916.1	6261.0	6543.3	6822.8	7059.7	1829.1
2002.9	3292.1	4099.9	4668.3	5165.1	5579.2	5925.9	6263.5	6546.9	6824.7	6958.1	1978.4
2059.0	3309.9	4109.2	4679.2	5167.5	5596.1	5925.9	6264.4	6548.1	6825.2	6968.5	2040.1
2078.7	3327.7	4143.1	4689.3	5172.2	5599.1	5940.4	6265.9	6555.1	6831.9	6970.4	2060.6
2112.2	3384.6	4149.2	4700.4	5176.7	5607.4	5943.0	6273.2	6561.7	6833.5	6984.0	2098.9
2138.3	3389.3	4173.5	4711.1	5189.8	5611.6	5947.0	6280.6	6575.4	6844.3	6985.3	2126.1
2162.9	3436.0	4181.5	4743.6	5202.9	5617.9	5948.4	6291.4	6577.7	6847.5	6993.3	2151.0
2164.5	3448.2	4188.1	4748.6	5208.1	5619.0	5953.9	6292.2	6584.8	6855.8	6995.5	2156.9
2193.4	3461.6	4197.7	4756.6	5216.3	5630.3	5964.3	6295.6	6587.9	6864.7	7001.4	2187.2
2228.7	3485.0	4224.3	4759.5	5216.6	5632.7	5976.3	6304.7	6592.4	6866.0	7011.2	2222.5
2254.2	3499.3	4231.0	4763.6	5239.6	5634.7	5980.6	6304.9	6599.0	6869.3	7011.4	2248.3
2335.0	3526.2	4240.7	4795.5	5243.4	5648.6	5989.8	6321.9	6605.1	6880.8	7022.3	2306.5
2391.1	3531.7	4254.3	4796.8	5249.3	5656.0	6000.8	6323.4	6605.4	6887.8	7024.8	2368.1
2407.2	3540.8	4263.7	4820.7	5260.4	5658.4	6010.9	6328.3	6613.8	6890.6	7032.7	2385.2
2443.7	3548.6	4272.2	4820.8	5277.2	5674.5	6013.5	6332.9	6619.8	6903.4	7035.9	2426.2
2466.5	3577.2	4276.9	4841.0	5281.3	5677.7	6014.2	6345.1	6624.6	6908.7	7038.0	2450.3
2488.3	3580.0	4283.5	4844.9	5287.1	5692.1	6026.2	6345.9	6625.5	6910.6	7038.6	2472.3
2494.8	3595.1	4305.8	4868.4	5294.1	5699.8	6032.4	6351.8	6628.8	6917.2	7045.4	2483.0
2520.4	3613.0	4314.4	4883.1	5297.3	5700.4	6033.4	6352.1	6635.7	6917.8	7047.4	2510.2
2553.6	3628.2	4323.6	4883.4	5297.4	5706.4	6033.9	6362.9	6641.0	6920.1	7055.6	2543.4
2576.7	3632.6	4343.8	4895.7	5315.9	5714.4	6049.6	6368.5	6641.6	6930.6	7059.7	2566.7
2666.5	3657.3	4353.4	4898.5	5330.2	5716.6	6057.4	6377.7	6652.2	6930.7		
2722.8	3668.6	4361.2	4918.1	5334.7	5718.6	6073.7	6386.0	6656.7	6931.2		
2735.1	3708.5	4365.4	4924.3	5340.5	5735.0	6074.9	6387.2	6665.7	6934.5		
2774.9	3714.6	4372.6	4924.4	5353.2	5738.1	6086.4	6392.3	6668.8	6941.1		
2794.2	3715.4	4396.5	4942.1	5359.0	5756.6	6093.6	6407.0	6672.1	6941.3		
2813.1	3722.6	4419.8	4957.2	5385.5	5761.0	6106.8	6409.6	6678.5	6946.3		
2825.0	3765.4	4424.7	4963.0	5386.3	5765.6	6106.8	6415.7	6685.9	6953.8		
2847.1	3774.4	4433.9	4965.7	5388.4	5776.4	6112.0	6418.0	6695.5	6954.4		

Table S8. Variationally calculated $\tilde{a}$ state vibrational energy levels of $C^{35}Cl_2$ and $C^{35}Cl^{37}Cl$.

$C^{35}Cl_2$	**$C^{35}Cl^{37}Cl$**
Var4	Var4
995.4	990.9
299.4	296.2
599.3	592.9
679.3	675.9
899.6	890.1
977.2	970.7
991.5	989.2
1200.4	1187.6
1275.6	1265.9
1286.8	1281.4
1352.0	1345.2
1501.8	1485.7
1574.5	1561.7
1582.5	1574.0
1648.4	1638.5
1666.2	1660.7