Supplementary material

I. Normalized cross section data

In the main body of the manuscript we present absolute cross sections for PT, DT and CT. For illustrating the relative importance of the rotation it is helpful to plot relative cross sections, here normalized to the values on the R(1) pump line, see Figures S1, S2 and S3.
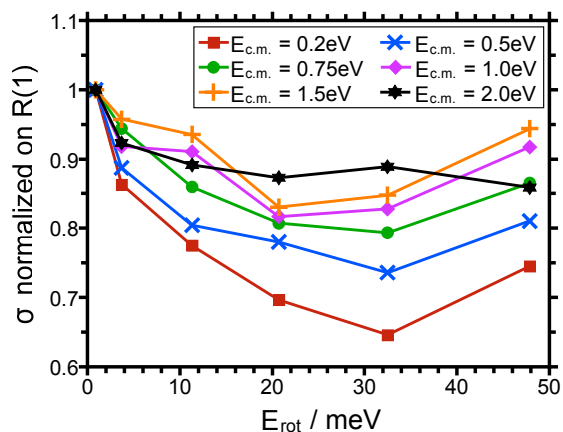

Figure S1   Normalized cross sections for proton transfer in the title reaction as a function of the average rotational energy, <E_{rot}>. The different traces correspond to different center of mass energies as indicated.

Figure S2   Normalized cross sections for deuteron transfer in the title reaction as a function of the average rotational energy, <E_{rot}>. The different traces correspond to different center of mass energies as indicated.

Figure S3   *Normalized cross sections for charge transfer in the title reaction as a function of the average rotational energy, <E_{rot}>. The different traces correspond to different center of mass energies as indicated.*
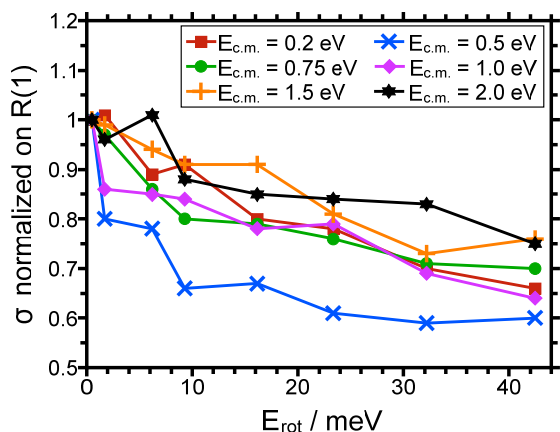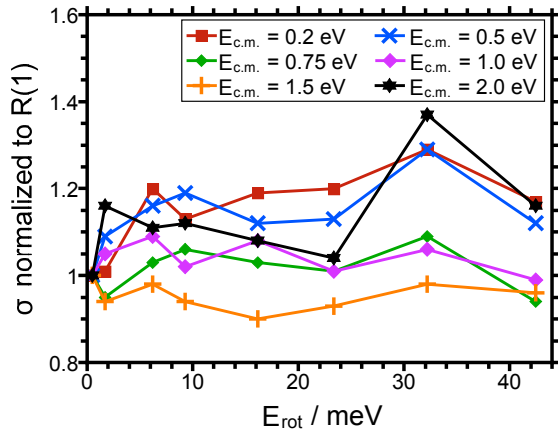
In particular for the PT shown in Figure S1 the rotational effect is clearly most pronounced at the lowest center of mass energy. The effect becomes smaller with increasing $E_{c.m.}$. For both PT and DT the relative variation of the cross section with E_{rot} is smallest for the highest $E_{c.m.}$. In the charge transfer the rotational dependence of the cross section is less pronounced. The local maximum of the cross section around E_{rot}=32.5 meV mentioned in the main text becomes evident in Figure S3 for all $E_{c.m.}$.

II.   Additional model calculations

In the main body of the manuscript we presented model calculation based on the concept of matching rotational velocities. We wish to point out that a slightly different approach in the model leads to smaller rms deviation, however at the cost of a larger number of parameters.

This alternative model is based on discussing the actual rotational energy of the ion (the rotational energy of the neutral is not explicitly taken into account). In this model the cross section is given by Equation (S1).

$$\sigma = a \cdot \left[E_{c.m.} + \frac{\left(\frac{E_{rot} + b}{B_0} \right)^2 + c}{d \cdot E_{c.m.}^e} \right]^f \quad\quad\quad (S1)$$

This model function can be rationalized as follows: The general form of Equation S1 resembles the classical form of the Langevin relation. However the energy operative has been corrected by a term containing the contribution of rotational energy, the 2nd summand in the bracket. As evident from looking at Figure of the main text the rotational dependence of the cross section exhibits a minimum around a rotational energy of 30 meV. Here, we assume that the rotational dependence of the cross

section can be modelled by an inverted parabola with 2 parameters for shifting in x- (b) and y- direction (c) respectively and a third parameter for the scaling of the parabola (d) . Further inspection of Figure (main text) reveals that the effect of the rotational correction depends on the center of mass collision energy, the correction being largest for the largest $E_{c.m.}$. Taking into account this effect requires another parameter (e).

By including the rotational constant we tried to generalize our proposed model function shown in Equation (S1). As a result we arrive at the fits included in Figure S4 and Figure S5. The optimized parameters are given in table S1

Figure S4   Cross sections for proton transfer in the title reaction as a function of the average rotational energy, $<E_{rot}>$. The different traces correspond to different center of mass energies as indicated.

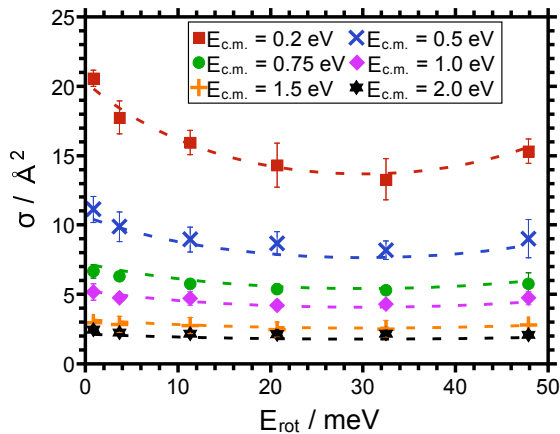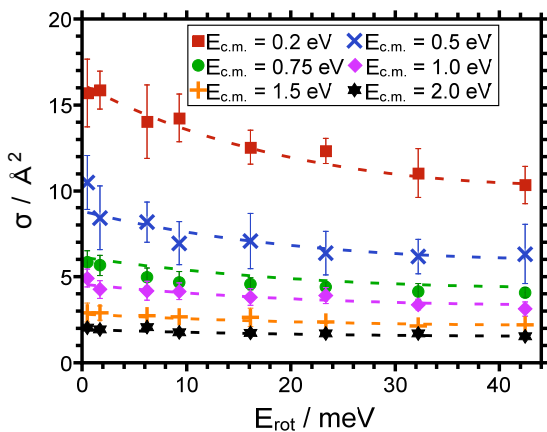*Figure S5   Cross sections for deuteron transfer in the title reaction as a function of the average rotational energy, $<E_{rot}>$. The different traces correspond to different center of mass energies as indicated.*

Table S1   Parameters obtained in the modeling of cross sections for PT and DT according to Equation (S1). The rotational constants are taken from ref. [1].

	PT	DT
a	26.129	
b	-0.03	-0.048
c	$-4.782*10^{-5}$	$-4.063*10^{-4}$
d	$-3.522*10^{-5}$	$-2.567*10^{-4}$
e	-0.105	
f	-2.164	
B_o	9.794 (HCl)	5.062 (DCl)

It is interesting to compare the optimized parameter sets. The fits described above used three parameters in common for simulating the PT and the DT data, i.e. the parameters a, e, and f.

The difference between the two parameter sets is observed in the values of b, c and d. We note, that b represents the rotational energy for which the cross section is minimum for a given collision energy. The parameter c reflects the shifting of the parabola on the sigma axis, i.e. the minimum value of sigma for a given collision energy. The parameter d reflects the scaling factor for the parabola accounting for the rotational correction. Evidently the model proposed is capable of describing the experimental data convincingly. Three parameters mainly affecting the collision energy dependence of σ are common to both data sets. Three parameters affecting the specific role of the rotational energy (or angular momentum) are specific for PT and DT. Note that we chose to include the rotational constant in the rotational term of equation (S1). Apparently this does not lead to a simplification of the model, but not to a complication either.

The form of the model function includes the possibility to account for a parabolic characteristic. This however, does not imply that the modelling is biased to this feature. As a matter of fact the data for DT are also well described by the model function although the data do not exhibit a minimum in the data range covered.

III. Geometry, energies and frequency parameters from ab initio calculations

S2 Geometry parameters on UMP2/def2-tzvpp, lengths in Å, angles in °

spezies	bond length / Å			bond angle / °		dihedral / °
1 - 2 - 3 - 4	1 - 2	2 - 3	3 - 4	1 - 2 - 3	2 - 3 - 4	1 - 2 - 3 - 4
HCl	1.26957	-	-	-	-	-
HCl$^+$	1.30869	-	-	-	-	-
HHCl$^+$	1.30026	1.30049	-	42.922	-	-
HClHCl (int1)	1.29005	2.89729	1.29005	97.333	61.222	-80.465
HClHCl (ts)	1.28390	1.97742	1.33968	99.414	124.010	-95.273
HClHCl (int2)	1.29185	1.42968	1.75246	94.942	178.273	180.000

S3 Geometry parameters on CCSD/def2-tzvpp, lengths in Å, angles in °

spezies	bond length / Å			bond angle / °		dihedral / °
1 - 2 - 3 - 4	1 - 2	2 - 3	3 - 4	1 - 2 - 3	2 - 3 - 4	1 - 2 - 3 - 4
HCl	1.27205	-	-	-	-	-
HCl$^+$	1.31085	-	-	-	-	-
HHCl$^+$	1.30119	1.30120	-	42.718	-	-
HClHCl (int1)	1.29079	2.91858	1.29079	97.419	61.148	-80.189
HClHCl (ts)	not optimizable with Gaussian 03					
HClHCl (int2)	1.29420	1.39154	1.85123	95.325	178.241	180.000

UMP2 / def2-tzvpp

S4 Energies on UMP2/def2-tzvpp in a.u.

energies in a.u.

	E	ZPVE	thermal	E + ZPVE
HCl	-460.30270	6.998E-03	-460.31356	-460.29570
HCl^+	-459.83973	6.264E-03	-459.84976	-459.83119
DCl	-460.30270	5.019E-03	-460.31621	-460.29768
DCl^+	-459.83973	4.493E-03	-459.85220	-459.83296
H_2Cl^+	-460.52338	1.558E-02	-460.52803	-460.50779
$HDCl^+$	-460.52338	1.341E-02	-460.53074	-460.50997
Cl	-459.63724	0.00	-459.65098	-459.63530
Cl^+	-459.16965	0.00	-459.18408	-459.16802
int1_HClHCl	-920.19761	1.659E-02	-920.20431	-920.17755
ts_HclHCl	-920.16670	1.433E-02	-920.17673	-920.15010
int2_HclHCl	-920.18156	1.529E-02	-920.19066	-920.16418
int1_DClHCl	-920.19761	1.434E-02	-920.20696	-920.17980
int1_HClDCl	-920.19761	1.434E-02	-920.20696	-920.17980
ts_DClHCl	-920.16670	1.211E-02	-920.17938	-920.15232
ts_HClDCl	-920.16670	1.264E-02	-920.17864	-920.15178
int2_DClHCl	-920.18156	1.302E-02	-920.19337	-920.16644
int2_HClDCl	-920.18156	1.339E-02	-920.19271	-920.16608

S5 Sum of electronic and thermal free energies in eV

	HCl	DCl1	DCl2
educts	0	0	0
int1	-1.115	-1.121	-1.121
ts	-0.365	-0.371	-0.350
int2	-0.744	-0.751	-0.733
products	-0.427	-0.434	-0.434
CT	-0.006		

S6 Sum of electronic and zero-point energies in eV

	HCl	DCl1	DCl2
educts	0	0	0
int1	-1.379	-1.392	-1.392
ts	-0.632	-0.644	-0.629
int2	-1.015	-1.028	-1.018
products	-0.441	-0.452	-0.452
CT	-0.006		

CCSD/def2-tzvpp

S7   Energies on CCSD/def2-tzvpp in a.u.

energies in a.u.

	E	ZPVE	thermal	E + ZPVE
HCl	-460.31590	6.912E-03	-460.33430	-460.31644
HCl$^+$	-459.85667	6.209E-03	-459.87563	-459.85706
DCl				
DCl$^+$				
H$_2$Cl$^+$	-460.53903	1.555E-02	-460.55159	-460.53135
HDCl$^+$				
Cl	-459.65283	0.00	-459.67456	-459.65888
Cl$^+$	-459.18764	0.00	-459.20908	-459.19302
int1_HClHCl	-920.21931	1.648E-02	-920.24575	-920.21896
ts_HclHCl	-920.19020	1.420E-02	-920.22256	-920.19593
int2_HclHCl	-920.20842	1.578E-02	-920.23413	-920.20748
int1_DClHCl				
int1_HClDCl				
ts_DClHCl				
ts_HClDCl				
int2_DClHCl				
int2_HClDCl				

S8   Sum of electronic and thermal free energies in eV

	HCl
educts	0
int1	-0.975
ts	-0.343
int2	-0.658
products	-0.441

S9   Sum of electronic and zero-point energies in eV

	HCl
educts	0
int1	-1.237
ts	-0.610
int2	-0.925
products	-0.456

CCSD(T)/def2-tzvpp // CCSD/def2-tzvpp

S10   Energies on CCSD(T)/def2-tzvpp // CCSD/def2-tzvpp in a.u.

energies in a.u.

	E	ZPVE	thermal	E + ZPVE
HCl	-460.32335	6.902E-03	-460.34223	-460.32436
HCl$^+$	-459.86326	6.202E-03	-459.88162	-459.86304
DCl	-460.32335	4.950E-03	-460.34484	-460.32631
DCl$^+$	-459.86326	4.448E-03	-459.88404	-459.86479
H$_2$Cl$^+$	-460.54691	1.550E-02	-460.55954	-460.53930
HDCl$^+$	-460.54691	1.334E-02	-460.56224	-460.54146
Cl	-459.65888	0.00	-459.68032	-459.66465
Cl$^+$	-459.19302	0.00	-459.21348	-459.19742
int1_HClHCl	-920.23533	1.624E-02	-920.26321	-920.23623
ts_HclHCl	-920.22724	1.402E-02	-920.23999	-920.21327
int2_HclHCl	-920.22326	1.569E-02	-920.24966	-920.22300
int1_DClHCl	-920.23533	1.402E-02	-920.26589	-920.23844
int1_HClDCl	-920.23533	1.404E-02	-920.26584	-920.23843
ts_DClHCl	-920.22724	1.186E-02	-920.24260	-920.21542
ts_HClDCl	-920.22724	1.234E-02	-920.24194	-920.21495
int2_DClHCl	-920.22326	1.345E-02	-920.25235	-920.22524
int2_HClDCl	-920.22326	1.364E-02	-920.25187	-920.22505

S11   Sum of electronic and thermal free energies in eV

	HCl	DCl1	DCl2
educts	0	0	0
int1	-1.071	-1.078	-1.077
ts	-0.439	-0.445	-0.427
int2	-0.702	-0.710	-0.697
products	-0.436	-0.443	-0.443
CT	-0.005		

S12   Sum of electronic and zero-point energies in eV

	HCl	DCl1	DCl2
educts	0	0	0
int1	-1.329	-1.341	-1.341
ts	-0.704	-0.715	-0.702
int2	-0.969	-0.982	-0.977
products	-0.450	-0.461	-0.461
CT	-0.005		

CCSD(T)/cc-pVTZ // CCSD/def2-tzvpp

S13   Energies on CCSD(T)/cc-pVTZ // CCSD/def2-tzvpp in a.u.

energies in a.u.

	E	ZPVE	thermal	E + ZPVE
HCl	-460.34	6.936E-03	-460.35	-460.33
HCl^+	-459.88	6.167E-03	-459.89	-459.87
DCl	-460.34	4.925E-03	-460.35	-460.33
DCl^+	-459.88	4.423E-03	-459.89	-459.87
H_2Cl^+	-460.56	1.555E-02	-460.56	-460.54
$HDCl^+$	-460.56	1.338E-02	-460.57	-460.55
Cl	-459.67	0.000E+00	-459.69	-459.67
Cl^+	-459.20	0.000E+00	-459.22	-459.20
int1_HClHCl	-920.26	1.614E-02	-920.27	-920.25
ts_HclHCl	-920.24	1.393E-02	-920.25	-920.23
int2_HclHCl	-920.25	1.553E-02	-920.26	-920.24
int1_DClHCl	-920.26	1.394E-02	-920.28	-920.25
int1_HClDCl	-920.26	1.395E-02	-920.28	-920.25
ts_DClHCl	-920.24	1.180E-02	-920.25	-920.23
ts_HClDCl	-920.24	1.224E-02	-920.25	-920.23
int2_DClHCl	-920.25	1.330E-02	-920.26	-920.24
int2_HClDCl	-920.25	1.352E-02	-920.26	-920.24

S14   Sum of electronic and thermal free energies in eV

	HCl	DCl1	DCl2
educts	0	0	0
int1	-1.061	-1.068	-1.067
ts	-0.446	-0.451	-0.435
int2	-0.712	-0.720	-0.706
products	-0.438	-0.446	-0.446
CT	-0.008		

S15   Sum of electronic and zero-point energies in eV

	HCl	DCl1	DCl2
educts	0	0	0
int1	-1.318	-1.331	-1.330
ts	-0.707	-0.718	-0.706
int2	-0.979	-0.992	-0.986
products	-0.452	-0.464	-0.464
CT	-0.008		

CCSD(T)/aug-cc-pVTZ // CCSD/def2-tzvpp

S16   Energies on CCSD(T)/aug-cc-pVTZ // CCSD/def2-tzvpp in a.u.

energies in a.u.

	E	ZPVE	thermal	E + ZPVE
HCl	-460.34321	6.944E-03	-460.35414	-460.33627
HCl$^+$	-459.87842	6.170E-03	-459.89083	-459.87225
DCl	-460.34324	4.931E-03	-460.35684	-460.33830
DCl$^+$	-459.87842	4.425E-03	-459.89324	-459.87399
H$_2$Cl$^+$	-460.56401	1.555E-02	-460.56870	-460.54846
HDCl$^+$	-460.56401	1.338E-02	-460.57141	-460.55063
Cl	-459.67622	0.00	-459.69189	-459.67622
Cl$^+$	-459.20669	0.00	-459.22275	-459.20669
int1_HClHCl	-920.27515	1.608E-02	-920.28637	-920.25924
ts_HclHCl	-920.25007	1.390E-02	-920.26314	-920.23625
int2_HclHCl	-920.26081	1.549E-02	-920.27199	-920.24532
int1_DClHCl	-920.27515	1.387E-02	-920.28911	-920.26145
int1_HClDCl	-920.27515	1.389E-02	-920.28902	-920.26143
ts_DClHCl	-920.25007	1.177E-02	-920.26575	-920.23837
ts_HClDCl	-920.25007	1.220E-02	-920.26518	-920.23794
int2_DClHCl	-920.26081	1.326E-02	-920.27468	-920.24755
int2_HClDCl	-920.26081	1.349E-02	-920.27417	-920.24733

S17   Sum of electronic and thermal free energies in eV

	HCl	DCl1	DCl2
educts	0	0	0
int1	-1.127	-1.136	-1.133
ts	-0.495	-0.500	-0.484
int2	-0.735	-0.743	-0.729
products	-0.425	-0.433	-0.433
CT	-0.008		

S18   Sum of electronic and zero-point energies in eV

	HCl	DCl1	DCl2
educts	0	0	0
int1	-1.380	-1.393	-1.392
ts	-0.755	-0.765	-0.753
int2	-1.002	-1.015	-1.009
products	-0.440	-0.451	-0.451
CT	-0.008		

S19   Harmonic vibrational frequencies in cm^{-1} for different spezies on UMP2 / def2-tzvpp

$HCl^+ + HCl \rightarrow H_2Cl^+ + Cl$
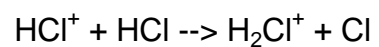
educts HCl$^+$	HClHCl (int1)	HClHCl (ts)	HClHCl (int2)	product H$_2$Cl$^+$
2749.6	199.0	-736.2	229.1	1218.5
	288.2	222.9	417.7	2802.4
HCl	493.9	306.7	666.3	2818.3
3071.6	508.8	520.3	1161.8	
	2892.2	2294.3	1353.5	
	2898.9	2943.7	2881.4	

S20   Rotational constants in GHz for different spezies on UMP2 / def2-tzvpp

HCl$^+$	HClHCl (int1)	HClHCl (ts)	HClHCl (int2)	H$_2$Cl$^+$
301.23	155.54	240.29	313.23	338.08
HCl				
	4.29	3.26	2.81	276.56
320.08	4.26	3.24	2.78	152.12

S21   Harmonic vibrational frequencies in cm^{-1} for different spezies on UMP2 / def2-tzvpp
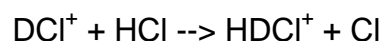
$DCl^+ + HCl \longrightarrow HDCl^+ + Cl$

educts DCl$^+$	DClHCl (int1-1)	HClDCl (int1-2)	DClHCl (ts-1)	HClDCl (ts-2)	DClHCl (int2-1)	HClDCl (int2-2)	product HDCl$^+$
1972.0	173.1	173.1	-735.7	-540.0	227.9	225.3	1060.6
	283.7	283.7	213.0	215.8	323.8	363.5	2015.9
HCl	365.2	365.2	252.9	266.6	666.3	474.7	2809.5
3071.6	501.3	501.3	443.1	477.4	1079.6	936.3	
	2076.9	2076.9	2110.7	1644.5	1351.6	996.0	
	2895.6	2895.6	2294.7	2943.6	2067.6	2880.8	

S22   Rotational constants in GHz for different spezies on UMP2 / def2-tzvpp

DCl$^+$	DClHCl (int1-1)	HClDCl (int1-2)	DClHCl (ts-1)	HClDCl (ts-2)	DClHCl (int2-1)	HClDCl (int2-2)	HDCl$^+$
154.95	105.80	105.80	142.27	191.57	161.55	313.23	311.29
HCl	4.22	4.22	3.20	3.24	2.76	2.81	154.39
320.08	4.15	4.15	3.15	3.23	2.72	2.78	103.20

S23   Harmonic vibrational frequencies in cm^{-1} for different spezies on CCSD / def2-tzvpp

$HCl^+ + HCl \rightarrow H_2Cl^+ + Cl$
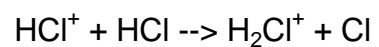
educts HCl^+	HClHCl (int1)	HClHCl (ts)	HClHCl (int2)	product H_2Cl^+
2725.6	197.1	-673.1	192.7	1232.9
	283.7	243.2	388.6	2789.0
HCl	483.2	282.4	620.1	2805.4
3034.0	513.8	491.2	1203.1	
	2872.0	2287.5	1666.1	
	2884.4	2930.7	2854.5	

S24   Rotational constants in GHz for different spezies on CCSD / def2-tzvpp

HCl^+	HClHCl (int1)	HClHCl (ts)	HClHCl (int2)	H_2Cl^+
300.24	155.45	240.29	312.65	340.32
HCl	4.23	3.26	2.70	274.35
318.83	4.21	3.24	2.68	151.90

S25   Harmonic vibrational frequencies in cm^{-1} for different spezies on CCSD(T) /def2-tzvpp // CCSD / def2-tzvpp
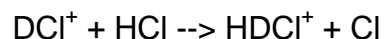
HCl$^+$ + HCl --> H$_2$Cl$^+$ + Cl
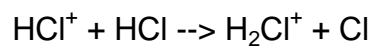
educts HCl$^+$		HClHCl (int1)	HClHCl (ts)	HClHCl (int2)	product H$_2$Cl$^+$
2722.3		148.3	-653.7	194.4	1216.4
		282.3	240.0	371.4	2786.7
HCl		459.6	244.0	606.8	2801.5
	3029.7	490.1	461.3	1186.1	
		2867.8	2282.8	1677.8	
		2879.5	2924.3	2850.7	

S26   Rotational constants in GHz for different spezies on CCSD(T) /def2-tzvpp // CCSD / def2-tzvpp

HCl$^+$		HClHCl (int1)	HClHCl (ts)	HClHCl (int2)	H$_2$Cl$^+$
300.24		155.45	240.29	312.65	340.32
HCl		4.23	3.26	2.70	274.35
	318.83	4.21	3.24	2.68	151.90

S27 Harmonic vibrational frequencies in cm^{-1} for different spezies on CCSD(T) /def2-tzvpp // CCSD / def2-tzvpp

DCl^{+} + HCl --> HDCl^{+} + Cl

educts DCl^{+}	DClHCl (int1-1)	HClDCl (int1-2)	DClHCl (ts-1)	HClDCl (ts-2)	DClHCl (int2-1)	HClDCl (int2-2)	product HDCl^{+}
1952.4	120.5	127.4	-652.7	-482.4	193.3	191.8	1057.7
	277.1	277.1	192.8	203.0	292.0	319.2	2003.5
HCl	346.0	346.0	241.9	232.9	606.7	432.3	2794.3
3029.7	475.9	476.0	392.6	419.2	1087.8	981.1	
	2060.9	2061.3	2097.0	1636.2	1676.2	1213.5	
	2874.0	2873.4	2283.0	2924.2	2046.2	2850.0	

S28 Rotational constants in GHz for different spezies on CCSD(T) /def2-tzvpp // CCSD / def2-tzvpp

DCl^{+}	DClHCl (int1-1)	HClDCl (int1-2)	DClHCl (ts-1)	HClDCl (ts-2)	DClHCl (int2-1)	HClDCl (int2-2)	HDCl^{+}
154.44	105.75	105.75	142.27	191.57	161.26	312.65	311.88
HCl	4.16	4.16	3.20	3.24	2.66	2.70	153.88
318.83	4.10	4.10	3.15	3.23	2.62	2.68	103.04

S29   Harmonic vibrational frequencies in cm^{-1} for different spezies on CCSD(T) / cc-pVTZ // CCSD / def2-tzvpp
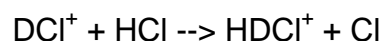
HCl$^+$ + HCl --> H$_2$Cl$^+$ + Cl
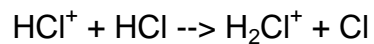
educts HCl$^+$		HClHCl (int1)	HClHCl (ts)	HClHCl (int2)	product H$_2$Cl$^+$
2707.1		145.0	-661.2	197.7	1205.8
		281.1	197.1	368.8	2804.7
HCl		455.2	242.7	602.9	2815.2
	3044.7	486.1	434.1	1173.6	
		2852.2	2301.9	1634.1	
		2864.2	2939.5	2839.8	

S30   Rotational constants in GHz for different spezies on CCSD(T) / cc-pVTZ // CCSD / def2-tzvpp

HCl$^+$		HClHCl (int1)	HClHCl (ts)	HClHCl (int2)	H$_2$Cl$^+$
298.29		154.57	240.29	311.20	340.32
HCl		4.21	3.26	2.71	274.35
	318.83	4.19	3.24	2.68	151.90

**S31** Harmonic vibrational frequencies in cm^{-1} for different spezies on CCSD(T) / cc-pVTZ // CCSD / def2-tzvpp

DCl$^+$ + HCl --> HDCl$^+$ + Cl

educts DCl$^+$	DClHCl (int1-1)	HClDCl (int1-2)	DClHCl (ts-1)	HClDCl (ts-2)	DClHCl (int2-1)	HClDCl (int2-2)	product HDCl$^+$
1941.5	117.8	124.3	-660.2	-487.4	196.7	195.1	1047.7
	276.1	276.1	159.3	158.3	289.7	317.1	2014.9
HCl	342.9	342.9	239.8	233.6	602.7	429.5	2810.2
3044.7	471.7	471.8	369.8	391.6	1076.8	969.9	
	2049.9	2050.2	2107.9	1649.9	1632.6	1182.7	
	2858.5	2857.9	2302.1	2939.4	2038.1	2839.3	

S32 Rotational constants in GHz for different spezies on CCSD(T) / cc-pVTZ // CCSD / def2-tzvpp

DCl$^+$	DClHCl (int1-1)	HClDCl (int1-2)	DClHCl (ts-1)	HClDCl (ts-2)	DClHCl (int2-1)	HClDCl (int2-2)	HDCl$^+$
153.43	105.16	105.16	142.27	191.57	160.52	311.20	311.88
HCl	4.14	4.14	3.20	3.24	2.66	2.71	153.88
318.83	4.08	4.08	3.15	3.23	2.62	2.68	103.04

S33 Harmonic vibrational frequencies in cm^{-1} for different spezies on CCSD(T) / aug-cc-pVTZ // CCSD / def2-tzvpp
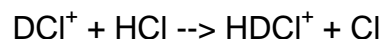
$HCl^+ + HCl \rightarrow H_2Cl^+ + Cl$
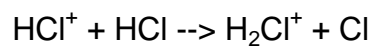
educts HCl$^+$		HClHCl (int1)	HClHCl (ts)	HClHCl (int2)	product H$_2$Cl$^+$
2708.4		121.6	-647.5	196.3	1205.1
		282.5	180.0	358.9	2806.0
HCl		451.6	245.7	591.8	2815.4
3048.3		480.2	425.5	1175.0	
		2854.9	2306.7	1636.0	
		2866.4	2942.7	2841.5	

S34 Rotational constants in GHz for different spezies on CCSD(T) / aug-cc-pVTZ // CCSD / def2-tzvpp

HCl$^+$	HClHCl (int1)	HClHCl (ts)	HClHCl (int2)	H$_2$Cl$^+$
298.29	154.57	240.29	311.20	340.32
HCl	4.21	3.26	2.71	274.35
318.83	4.19	3.24	2.68	151.90

S35 Harmonic vibrational frequencies in cm^{-1} for different spezies on CCSD(T) / aug-cc-pVTZ // CCSD / def2-tzvpp

DCl$^+$ + HCl --> HDCl$^+$ + Cl

educts DCl$^+$	DClHCl (int1-1)	HClDCl (int1-2)	DClHCl (ts-1)	HClDCl (ts-2)	DClHCl (int2-1)	HClDCl (int2-2)	product HDCl$^+$
1942.5	92.1	100.6	-646.4	-478.1	195.3	193.7	1046.7
	277.7	277.7	146.2	140.1	282.2	308.6	2015.4
HCl	339.5	339.5	241.9	236.2	591.7	421.6	2811.0
3048.3	466.8	466.9	361.6	383.5	1077.5	971.2	
	2051.6	2052.0	2110.2	1653.3	1634.7	1184.0	
	2861.0	2860.4	2306.9	2942.7	2039.2	2840.9	

S36 Rotational constants in GHz for different spezies on CCSD(T) / aug-cc-pVTZ // CCSD / def2-tzvpp

DCl$^+$	DClHCl (int1-1)	HClDCl (int1-2)	DClHCl (ts-1)	HClDCl (ts-2)	DClHCl (int2-1)	HClDCl (int2-2)	HDCl$^+$
153.43	105.16	105.16	142.27	191.57	160.52	311.20	311.88
HCl							
	4.14	4.14	3.20	3.24	2.66	2.71	153.88
318.83	4.08	4.08	3.15	3.23	2.62	2.68	103.04

IV.   Comparison of relevant orbiting and rotational angular momenta

Tables S37 Rotational angular momenta of the HCl$^+$

Pump line	N /(kg*m^2*s^{-1})	N / ℏ
R(1)	4.463E-35	0.4232
R(2)	1.529E-34	1.4503
R(3)	3.060E-34	2.9019
R(4)	4.225E-34	4.0063
R(5)	5.340E-34	5.0639
R(6)*	6.665E-34	6.3203

* extrapolated

Table S38   Orbiting angular momenta of the HCl$^+$ + HCl system

E$_{c.m.}$ / eV	L /(kg*m^2*s^{-1})	L / ℏ
0.2	1.957E-32	185.561
0.5	2.461E-32	233.331
0.75	2.723E-32	258.223
1.0	2.926E-32	277.479
1.5	3.238E-32	307.081
2.0	3.480E-32	329.980

Table S39   Rotational angular momenta of the DCl$^+$

Pump line	N /(kg*m^2*s^{-1})	N / ℏ
R(1)	5.020E-35	0.4760
R(2)	1.351E-34	1.2814
R(3)	3.034E-34	2.8773
R(4)	3.875E-34	3.6746
R(5)	5.245E-34	4.9738
R(6)*	6.405E-34	6.0733
R(7)*	7.606E-34	7.2122
R(8)*	8.807E-34	8.3511

* extrapolated

Table S40   Orbiting angular momenta of the DCl$^+$ + HCl system

E$_{c.m.}$ / eV	L /(kg*m^2*s^{-1})	L / ℏ
0.2	1.970E-32	186.811
0.5	2.477E-32	234.902
0.75	2.741E-32	259.962
1.0	2.946E-32	279.348
1.5	3.260E-32	309.149
2.0	3.503E-32	332.202

Literature

1   K. L. Saenger, R. N. Zare and C. Mathews, *Journal of Molecular Spectroscopy*, 1976, **61**, 216–230.