

Supporting Information

Can a gas phase contact ion pair containing a hydrocarbon carbocation be formed in the ground state?

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Additional analysis of the three H bonds of the HBCIP

Based on the elongations due to the interaction with the Cl atom (~ 0.019 Å for the central and ~ 0.005 Å for the remaining two H bonds), it is clear that the central H bond is considerably stronger. Although the present study is not intended to give a complete description of the nature of these three H bonds, below it is shown that they satisfy most of the criteria recommended by the IUPAC [1, section 2.1]:

For a hydrogen bond $X-H\cdots Y-Z$:

(E1) The forces involved in the formation of a hydrogen bond include those of an electrostatic origin, those arising from charge transfer between the donor and acceptor leading to partial covalent bond formation between H and Y, and those originating from dispersion.

The electrostatic origin of the bond is clear, due to the charge transfer in the $C^+-H\cdots Cl^-$ motif. Besides, there should be a significant covalent character in the H bond, as the $H\cdots Cl^-$ distance (2.096 Å, see Figure 1) is considerably smaller than the sum of the van der Waals radii of H and Cl^- [2] ($1.2 + 3.50 = 4.70$ Å).

(E2) The atoms X and H are covalently bonded to one another and the X–H bond is polarized, the H–Y bond strength increasing with the increase in electronegativity of X.

Clearly the partial positive charge on the central C atom leads to a significant polarization of the covalent C^+-H bond, which can be confirmed by its elongation, as compared to the corresponding bond length in the radical (~ 1.102 versus 1.082 Å). Due to the resonance within the fused rings, a partial positive charge is also expected for the adjacent C atoms. Besides, this charge should be larger than the corresponding charge in the radical, again leading to some polarization of the other two covalent C–H bonds which also form H bonds, but the effect is significantly smaller, as it leads to an elongation of only ~ 0.005 Å for these bonds.

Analysis of the other hypothesis requires comparison of H bonds containing the same $A^+-H\cdots Cl^-$ motif but varying the electronegativity of A (for instance, from $C \rightarrow Si \rightarrow Ge$), but ideally maintaining the same number of bonds with A.

(E3) The $X-H\cdots Y$ angle is usually linear (180°) and the closer the angle is to 180° , the stronger is the hydrogen bond and the shorter is the $H\cdots Y$ distance.

As shown in Figure 1, the $C^+-H\cdots Cl^-$ angle of the central C atom is 180° , while the corresponding angle of the other two H bonds is 146.3° , which is consistent with two weaker H bonds.

(E4) The length of the X–H bond usually increases on hydrogen bond formation leading to a red shift in the infrared X–H stretching frequency and an increase in the infrared absorption cross-section for the X–H stretching vibration. The greater the lengthening of the X–H bond in $X-H\cdots Y$, the stronger is the $H\cdots Y$ bond. Simultaneously, new vibrational modes associated with the formation of the $H\cdots Y$ bond are generated.

As discussed above and in the manuscript (just before the suggested mechanism), the three mentioned C–H bonds increase on H bond formation. As also discussed in the same paragraph of the

manuscript, one has a relatively large red shift of $\sim 200\text{ cm}^{-1}$, for the C–H bonds involved in the H bond. Actually one has three H bonds and, although this vibrational mode is much more localized on the central $\text{C}^+-\text{H}\cdots\text{Cl}^-$ moiety, its visualization also indicates a small contribution of the adjacent C–H bonds. At all computational levels the intensity of this mode is by far the largest one. Among the new intermolecular modes associated with H bond formation (in the far infrared region), the most important one is that with a frequency of $\sim 160\text{ cm}^{-1}$, as it has the highest intensity in this region and thus it can also be used to identify the HBCIP, as also discussed in the paragraph just before the suggested mechanism.

(E5) The $\text{X}-\text{H}\cdots\text{Y}-\text{Z}$ hydrogen bond leads to characteristic NMR signatures that typically include pronounced proton deshielding for H in $\text{X}-\text{H}$, through hydrogen bond spin–spin couplings between X and Y, and nuclear Overhauser enhancements.

Although not mentioned in the manuscript, NMR spectroscopy in principle can also be used to identify the HBCIP trapped in He nanodroplets, but it seems that the experimental setup is very difficult [3].

(E6) The Gibbs energy of formation for the hydrogen bond should be greater than the thermal energy of the system for the hydrogen bond to be detected experimentally.

In the case of the HBCIP studied in this work this statement should be adapted, replacing the Gibbs energy of formation for the hydrogen bond by the $\text{HBCIP} \rightarrow \text{TS1}$ free energy barrier, as it is assumed that the experimental setup is able to kinetically trap the HBCIP. Besides, with this trap its thermal energy becomes that of the He nanodroplet, $3RT/2$. For $T = 0.4\text{K}$, $3RT/2 \sim 1.2 \times 10^{-3}\text{ kcal/mol}$. For a free energy barrier of $\sim 1.0\text{ kcal/mol}$ (the lowest value obtained) the requirement is easily satisfied.

Table S1. Cartesian coordinates (in Å) of the structures optimized at the M05-2X/6-31++G** level.

radical				cation			
C -3.70725800	-1.15612300	0.00000000	C 1.18113400	3.66925700	0.00000000		
C -2.38332100	-1.55229000	0.00000000	C 1.56991900	2.35587200	0.00000000		
C -1.31037500	-0.62605900	0.00000000	C 0.61642300	1.29304800	0.00000000		
C -1.64130100	0.75899200	0.00000000	C -0.78078200	1.62170700	0.00000000		
C -2.99240100	1.13411700	0.00000000	C -1.14277600	2.98701300	0.00000000		
C -4.02275400	0.20500000	0.00000000	C -0.19371300	3.98502900	0.00000000		
C 0.00000000	-1.18859600	0.00000000	C 1.16406300	0.00000000	0.00000000		
C 1.64143900	0.75885600	0.00000000	C -0.78078200	-1.62170700	0.00000000		
C 1.31039800	-0.62615400	0.00000000	C 0.61642300	-1.29304800	0.00000000		
C 2.38302000	-1.55284000	0.00000000	C 1.56991900	-2.35587200	0.00000000		
H 2.14369700	-2.60979800	0.00000000	H 2.62333400	-2.10439100	0.00000000		
C 3.70700000	-1.15654800	0.00000000	C 1.18113500	-3.66925700	0.00000000		
C 4.02277000	0.20451000	0.00000000	C -0.19371300	-3.98502900	0.00000000		
C 2.99257600	1.13379800	0.00000000	C -1.14277600	-2.98701300	0.00000000		
H -4.49344600	-1.90090000	0.00000000	H 1.92002900	4.45934500	0.00000000		
H -2.14426300	-2.60903800	0.00000000	H 2.62333400	2.10439100	0.00000000		
H -3.22958500	2.19193000	0.00000000	H -2.19409300	3.24522700	0.00000000		
H -5.05412100	0.53333800	0.00000000	H -0.50647900	5.02150700	0.00000000		
H 4.49312100	-1.90141200	0.00000000	H 1.92003000	-4.45934500	0.00000000		
H 5.05418500	0.53270700	0.00000000	H -0.50648000	-5.02150700	0.00000000		
H 3.22992300	2.19157700	0.00000000	H -2.19409200	-3.24522700	0.00000000		
C -0.67334800	1.84697100	0.00000000	C -1.85389900	0.68260900	0.00000000		
C 0.67359900	1.84692500	0.00000000	C -1.85389900	-0.68260900	0.00000000		
H -0.00008400	-2.27239000	0.00000000	H 2.24997000	0.00000000	0.00000000		
H -1.13297100	2.83035500	0.00000000	H -2.83780900	1.13841300	0.00000000		
H 1.13328500	2.83028200	0.00000000	H -2.83781000	-1.13841300	0.00000000		
HBCIP			HBCIP (with BSSE)				
C 0.00000000	3.65208600	0.56748500	C 0.00000000	3.65252000	0.56689900		
C 0.00000000	2.32991100	0.94759200	C 0.00000000	2.33040600	0.94721800		
C 0.00000000	1.29204400	-0.02870500	C 0.00000000	1.29192400	-0.02849200		
C 0.00000000	1.62569900	-1.41879300	C 0.00000000	1.62558000	-1.41858100		
C 0.00000000	2.99013300	-1.76676600	C 0.00000000	2.98989700	-1.76699600		
C 0.00000000	3.97780200	-0.79956600	C 0.00000000	3.97799000	-0.80022000		
C 0.00000000	0.00000000	0.52981500	C 0.00000000	0.00000000	0.53050500		
C 0.00000000	-1.62569900	-1.41879300	C 0.00000000	-1.62558000	-1.41858100		
C 0.00000000	-1.29204400	-0.02870500	C 0.00000000	-1.29192400	-0.02849200		
C 0.00000000	-2.32991100	0.94759200	C 0.00000000	-2.33040600	0.94721800		
H 0.00000000	-2.03129000	1.99449900	H 0.00000000	-2.03298500	1.99436900		
C 0.00000000	-3.65208600	0.56748500	C 0.00000000	-3.65252000	0.56689900		
C 0.00000000	-3.97780200	-0.79956600	C 0.00000000	-3.97799000	-0.80022000		
C 0.00000000	-2.99013300	-1.76676600	C 0.00000000	-2.98989700	-1.76699600		
H 0.00000000	4.43391200	1.31529100	H 0.00000000	4.43447500	1.31454600		
H 0.00000000	2.03129000	1.99449900	H 0.00000000	2.03298500	1.99436900		
H 0.00000000	3.26289000	-2.81502600	H 0.00000000	3.26210300	-2.81538600		
H 0.00000000	5.01756300	-1.10351600	H 0.00000000	5.01766800	-1.10443900		
H 0.00000000	-4.43391200	1.31529100	H 0.00000000	-4.43447500	1.31454600		
H 0.00000000	-5.01756300	-1.10351600	H 0.00000000	-5.01766800	-1.10443900		
H 0.00000000	-3.26289000	-2.81502600	H 0.00000000	-3.26210300	-2.81538600		
C 0.00000000	0.68024000	-2.49739400	C 0.00000000	0.68017400	-2.49756500		

C 0.00000000 -0.68024000 -2.49739400	C 0.00000000 -0.68017400 -2.49756500
CI 0.00000000 0.00000000 3.72474000	CI 0.00000000 0.00000000 3.72580900
H 0.00000000 0.00000000 1.63337500	H 0.00000000 0.00000000 1.63440300
H 0.00000000 1.13874500 -3.48078100	H 0.00000000 1.13907200 -3.48075300
H 0.00000000 -1.13874500 -3.48078100	H 0.00000000 -1.13907200 -3.48075300
TS1	TS1 (with BSSE)
C 0.59886800 -0.28791000 3.66288900	C 0.59739100 -0.28977300 3.66279700
C 0.96677700 -0.41821900 2.34415400	C 0.96547700 -0.41909100 2.34404900
C 0.01853700 -0.25880700 1.29597200	C 0.01729600 -0.25827200 1.29590300
C -1.33285500 0.06175100 1.62203400	C -1.33419100 0.06218300 1.62215600
C -1.67695800 0.17207000 2.98435100	C -1.67831600 0.17184900 2.98451700
C -0.73811800 0.00205400 3.98237200	C -0.73955000 0.00053300 3.98236300
C 0.55513100 -0.45038700 0.00000000	C 0.55399300 -0.44817500 0.00000000
C -1.33285500 0.06175100 -1.62203400	C -1.33419100 0.06218300 -1.62215600
C 0.01853700 -0.25880700 -1.29597200	C 0.01729600 -0.25827200 -1.29590300
C 0.96677700 -0.41821900 -2.34415400	C 0.96547700 -0.41909100 -2.34404900
H 2.00181200 -0.57732000 -2.06032200	H 2.00054800 -0.57910300 -2.06059700
C 0.59886800 -0.28791000 -3.66288900	C 0.59739100 -0.28977300 -3.66279700
C -0.73811800 0.00205400 -3.98237200	C -0.73955000 0.00053300 -3.98236300
C -1.67695800 0.17207000 -2.98435100	C -1.67831600 0.17184900 -2.98451700
H 1.33761500 -0.39389700 4.44607600	H 1.33589400 -0.39700700 4.44602400
H 2.00181200 -0.57732000 2.06032200	H 2.00054800 -0.57910300 2.06059700
H -2.70246100 0.40440000 3.24404500	H -2.70368900 0.40452800 3.24437900
H -1.03537400 0.10571800 5.01859800	H -1.03679500 0.10351800 5.01866300
H 1.33761500 -0.39389700 -4.44607600	H 1.33589400 -0.39700700 -4.44602400
H -1.03537400 0.10571800 -5.01859800	H -1.03679500 0.10351800 -5.01866300
H -2.70246100 0.40440000 -3.24404500	H -2.70368900 0.40452800 -3.24437900
C -2.39702300 0.26347200 0.67859800	C -2.39781900 0.26559900 0.67865000
C -2.39702300 0.26347200 -0.67859800	C -2.39781900 0.26559900 -0.67865000
CI 3.37221200 0.53412500 0.00000000	CI 3.37961800 0.53429400 0.00000000
H 1.58647800 -0.78508600 0.00000000	H 1.58710800 -0.77773700 0.00000000
H -3.35939000 0.45828000 1.13977200	H -3.35997300 0.46178500 1.13968600
H -3.35939000 0.45828000 -1.13977200	H -3.35997300 0.46178500 -1.13968600
TS2	cov1
C -3.76753800 0.66443900 -0.08933300	C 0.69492900 -1.29847300 3.41936100
C 3.76753800 0.66443900 -0.08933300	C 1.22247500 -0.91268700 2.19313500
C -2.46690800 1.10570000 0.11607400	C 0.46095300 -0.19181900 1.27012700
C 2.46690800 1.10570000 0.11607400	C -0.86951100 0.14187000 1.57934600
C -1.36140800 0.24100200 0.15856000	C -1.37677800 -0.22730900 2.83450900
C 1.36140800 0.24100200 0.15856000	C -0.61341000 -0.94465800 3.74458700
C -1.62539300 -1.13860600 0.03812900	C 1.12750600 0.25098400 0.00000000
C 1.62539300 -1.13860600 0.03812900	C -0.86951100 0.14187000 -1.57934600
C -2.94946700 -1.56745200 -0.17774400	C 0.46095300 -0.19181900 -1.27012700
C 2.94946700 -1.56745200 -0.17774400	C 1.22247500 -0.91268700 -2.19313500
C -4.01697900 -0.69210700 -0.25562000	H 2.25020200 -1.15778900 -1.94991200
C 4.01697900 -0.69210700 -0.25562000	C 0.69492900 -1.29847300 -3.41936100
C 0.00000000 0.87341500 0.50280300	C -0.61341000 -0.94465800 -3.74458700
H 2.31425300 2.16464400 0.24776600	C -1.37677800 -0.22730900 -2.83450900
H -2.31425300 2.16464400 0.24776600	H 1.30442200 -1.85297600 4.12154600
H -4.57489900 1.38526800 -0.11481800	H 2.25020200 -1.15778900 1.94991200
H 4.57489900 1.38526800 -0.11481800	H -2.39616600 0.04538700 3.08274000

H -3.12540500	-2.63132900	-0.28302300	H -1.03396500	-1.22437000	4.70233200
H 3.12540500	-2.63132900	-0.28302300	H 1.30442200	-1.85297600	-4.12154600
H -5.02006000	-1.06152400	-0.42674600	H -1.03396500	-1.22437000	-4.70233200
H 5.02006000	-1.06152400	-0.42674600	H -2.39616600	0.04538700	-3.08274000
C -0.66844400	-2.23506600	0.15144700	C -1.76889200	0.85445800	0.67238500
C 0.66844300	-2.23506600	0.15144700	C -1.76889200	0.85445800	-0.67238500
Cl 0.00000000	2.58077000	-0.18713100	H -2.58287300	1.37971500	1.16169300
H 0.00000000	1.05924800	1.57863900	H -2.58287300	1.37971500	-1.16169300
H -1.13665200	-3.21093300	0.22063000	H 2.14615100	-0.12847200	0.00000000
H 1.13665200	-3.21093300	0.22063000	Cl 1.35343300	2.06976800	0.00000000
cov2					
C -0.51886100	1.23060400	3.23403100			
C -1.06187900	0.68065300	2.07802000			
C -0.28473200	-0.12023800	1.24260800			
C 1.06758800	-0.34874700	1.55447400			
C 1.58798000	0.18191000	2.74392100			
C 0.80751800	0.97045400	3.57664900			
C -0.81235200	-0.80130700	0.00000000			
C 1.06758800	-0.34874700	-1.55447400			
C -0.28473200	-0.12023800	-1.24260800			
C -1.06187900	0.68065300	-2.07802000			
H -2.10127900	0.85187800	-1.83334400			
C -0.51886100	1.23060400	-3.23403100			
C 0.80751800	0.97045400	-3.57664900			
C 1.58798000	0.18191000	-2.74392100			
H -1.13723600	1.84458200	3.87674700			
H -2.10127900	0.85187800	1.83334400			
H 2.62367500	-0.01629800	2.99561500			
H 1.22814500	1.38105700	4.48582000			
H -1.13723600	1.84458200	-3.87674700			
H 1.22814500	1.38105700	-4.48582000			
H 2.62367500	-0.01629800	-2.99561500			
C 1.97094900	-1.09817700	0.67416000			
C 1.97094900	-1.09817700	-0.67416000			
H 2.78482900	-1.61604400	1.17203700			
H 2.78482900	-1.61604400	-1.17203700			
Cl -2.60571000	-0.95356500	0.00000000			
H -0.44781900	-1.82940600	0.00000000			

Table S2. Cartesian coordinates (in Å) of the structures optimized at the M05-2X/6-311++G**(H,Cl)/6-31++G**(C) level.

HBCIP				HBCIP (with BSSE)			
C	0.00000000	3.65294000	0.56598200	C	0.00000000	3.65313800	0.56508900
C	0.00000000	2.33097000	0.94662400	C	0.00000000	2.33126700	0.94592200
C	0.00000000	1.29212000	-0.02843600	C	0.00000000	1.29218400	-0.02900700
C	0.00000000	1.62551100	-1.41887300	C	0.00000000	1.62551300	-1.41947800
C	0.00000000	2.98978000	-1.76741700	C	0.00000000	2.98976900	-1.76825100
C	0.00000000	3.97819300	-0.80108200	C	0.00000000	3.97822800	-0.80208100
C	0.00000000	0.00000000	0.52991200	C	0.00000000	0.00000000	0.52927400
C	0.00000000	-1.62551100	-1.41887300	C	0.00000000	-1.62551300	-1.41947800
C	0.00000000	-1.29212000	-0.02843600	C	0.00000000	-1.29218400	-0.02900700
C	0.00000000	-2.33097000	0.94662400	C	0.00000000	-2.33126700	0.94592200
H	0.00000000	-2.03528000	1.99335700	H	0.00000000	-2.03591300	1.99277100
C	0.00000000	-3.65294000	0.56598200	C	0.00000000	-3.65313800	0.56508900
C	0.00000000	-3.97819300	-0.80108200	C	0.00000000	-3.97822800	-0.80208100
C	0.00000000	-2.98978000	-1.76741700	C	0.00000000	-2.98976900	-1.76825100
H	0.00000000	4.43451400	1.31298200	H	0.00000000	4.43495300	1.31182600
H	0.00000000	2.03528000	1.99335700	H	0.00000000	2.03591300	1.99277100
H	0.00000000	3.26103900	-2.81524100	H	0.00000000	3.26075700	-2.81612600
H	0.00000000	5.01713600	-1.10541700	H	0.00000000	5.01716800	-1.10643900
H	0.00000000	-4.43451400	1.31298200	H	0.00000000	-4.43495300	1.31182600
H	0.00000000	-5.01713600	-1.10541700	H	0.00000000	-5.01716800	-1.10643900
H	0.00000000	-3.26103900	-2.81524100	H	0.00000000	-3.26075700	-2.81612600
C	0.00000000	0.68022900	-2.49732200	C	0.00000000	0.68021900	-2.49792400
C	0.00000000	-0.68022900	-2.49732200	C	0.00000000	-0.68021900	-2.49792400
Cl	0.00000000	0.00000000	3.72843800	Cl	0.00000000	0.00000000	3.73286800
H	0.00000000	0.00000000	1.63205000	H	0.00000000	0.00000000	1.63151700
H	0.00000000	1.13876900	-3.48002400	H	0.00000000	1.13878200	-3.48060900
H	0.00000000	-1.13876900	-3.48002400	H	0.00000000	-1.13878200	-3.48060900
TS1				TS1 (with BSSE)			
C	-0.59478800	-0.28409300	-3.66242400	C	0.59345300	-0.28852300	3.66250100
C	-0.96329000	-0.41161500	-2.34362000	C	0.96181400	-0.41641700	2.34374200
C	-0.01370200	-0.25378100	-1.29592800	C	0.01288200	-0.25553300	1.29592300
C	1.33935900	0.06140600	-1.62256300	C	-1.33959100	0.06239000	1.62258300
C	1.68329700	0.16939600	-2.98493800	C	-1.68347100	0.17066500	2.98498000
C	0.74311600	0.00166400	-3.98215400	C	-0.74382000	0.00034900	3.98221100
C	-0.55062300	-0.43653400	0.00000000	C	0.54986900	-0.43751100	0.00000000
C	1.33935900	0.06140600	1.62256300	C	-1.33959100	0.06239000	-1.62258300
C	-0.01370200	-0.25378100	1.29592800	C	0.01288200	-0.25553300	-1.29592300
C	-0.96329000	-0.41161500	2.34362000	C	0.96181400	-0.41641700	-2.34374200
H	-1.99781800	-0.57074100	2.06020300	H	1.99606400	-0.57823900	-2.06080300
C	-0.59478800	-0.28409300	3.66242400	C	0.59345300	-0.28852300	-3.66250100
C	0.74311600	0.00166400	3.98215400	C	-0.74382000	0.00034900	-3.98221100
C	1.68329700	0.16939600	2.98493800	C	-1.68347100	0.17066500	-2.98498000
H	-1.33283100	-0.39017400	-4.44526200	H	1.33115700	-0.39675100	4.44534800
H	-1.99781800	-0.57074100	-2.06020300	H	1.99606400	-0.57823900	2.06080300
H	2.70879800	0.39782200	-3.24474100	H	-2.70845700	0.40141400	3.24473500
H	1.04002000	0.10301900	-5.01798800	H	-1.04056900	0.10209600	5.01804600
H	-1.33283100	-0.39017400	4.44526200	H	1.33115700	-0.39675100	-4.44534800

H 1.04002000 0.10301900 5.01798800	H -1.04056900 0.10209600 -5.01804600
H 2.70879800 0.39782200 3.24474100	H -2.70845700 0.40141400 -3.24473500
C 2.40296200 0.26077300 -0.67879200	C -2.40255200 0.26485900 0.67882200
C 2.40296200 0.26077300 0.67879200	C -2.40255200 0.26485900 -0.67882200
Cl -3.40226500 0.52121700 0.00000000	Cl 3.40592700 0.52629200 0.00000000
H -1.58834600 -0.75227400 0.00000000	H 1.58798800 -0.75188800 0.00000000
H 3.36540000 0.45296100 -1.13956700	H -3.36446300 0.45973300 1.13956300
H 3.36540000 0.45296100 1.13956700	H -3.36446300 0.45973300 -1.13956300
TS2	cov1
C -3.76737100 0.66411000 -0.09432700	C 0.70280400 -1.29332700 3.42049700
C -2.46701200 1.10577000 0.11198600	C 1.22769400 -0.90635200 2.19353200
C -1.36126700 0.24142800 0.15815700	C 0.46215200 -0.18995500 1.27043600
C -1.62528800 -1.13846600 0.03853400	C -0.86976500 0.13777100 1.58017200
C -2.94917500 -1.56780500 -0.17700100	C -1.37437800 -0.23270900 2.83604900
C -4.01672200 -0.69274400 -0.25752300	C -0.60698200 -0.94555600 3.74625800
C 0.00000000 0.87260700 0.50309300	C 1.12472300 0.25584900 0.00000000
C 1.62528800 -1.13846600 0.03853400	C -0.86976500 0.13777100 -1.58017200
C 1.36126700 0.24142800 0.15815700	C 0.46215200 -0.18995500 -1.27043600
C 2.46701200 1.10577000 0.11198600	C 1.22769400 -0.90635200 -2.19353200
H 2.31577600 2.16419900 0.24173600	H 2.25556000 -1.14647500 -1.94968500
C 3.76737100 0.66411000 -0.09432700	C 0.70280400 -1.29332700 -3.42049700
C 4.01672200 -0.69274400 -0.25752300	C -0.60698200 -0.94555600 -3.74625800
C 2.94917500 -1.56780500 -0.17700100	C -1.37437800 -0.23270900 -2.83604900
H -4.57414100 1.38430400 -0.12231200	H 1.31474300 -1.84410900 4.12224900
H -2.31577600 2.16419900 0.24173600	H 2.25556000 -1.14647500 1.94968500
H -3.12463200 -2.63106700 -0.27987600	H -2.39416400 0.03505300 3.08421100
H -5.01900400 -1.06231900 -0.42814300	H -1.02501100 -1.22629700 4.70391600
H 4.57414100 1.38430300 -0.12231200	H 1.31474300 -1.84410900 -4.12224900
H 5.01900400 -1.06231900 -0.42814300	H -1.02501100 -1.22629700 -4.70391600
H 3.12463200 -2.63106700 -0.27987600	H -2.39416400 0.03505300 -3.08421100
C -0.66843000 -2.23440700 0.15431800	C -1.77344100 0.84352900 0.67241400
C 0.66843000 -2.23440800 0.15431800	C -1.77344100 0.84352900 -0.67241400
Cl 0.00000000 2.58123100 -0.18109900	Cl 1.33945600 2.07421400 0.00000000
H 0.00000000 1.05762100 1.57744700	H 2.14428600 -0.11658100 0.00000000
H -1.13632000 -3.20951600 0.22507300	H -2.59133000 1.36134600 1.16130200
H 1.13632000 -3.20951600 0.22507300	H -2.59133000 1.36134600 -1.16130200
cov2	
C -0.52035900 1.22804500 3.23727600	
C -1.06238400 0.68052100 2.07967700	
C -0.28457300 -0.11823600 1.24280100	
C 1.06747300 -0.34745900 1.55538500	
C 1.58687300 0.18076100 2.74643800	
C 0.80573400 0.96725800 3.58038400	
C -0.81128500 -0.79843600 0.00000000	
C 1.06747300 -0.34745900 -1.55538500	
C -0.28457300 -0.11823600 -1.24280100	
C -1.06238400 0.68052100 -2.07967700	
H -2.10095500 0.85189900 -1.83552400	
C -0.52035900 1.22804500 -3.23727600	
C 0.80573400 0.96725800 -3.58038400	
C 1.58687300 0.18076100 -2.74643800	

H	-1.13876300	1.84028300	3.88035100
H	-2.10095500	0.85189900	1.83552400
H	2.62158600	-0.01824700	2.99780400
H	1.22504200	1.37546000	4.49033100
H	-1.13876300	1.84028300	-3.88035100
H	1.22504200	1.37546000	-4.49033100
H	2.62158600	-0.01824700	-2.99780400
C	1.97182900	-1.09403100	0.67411500
C	1.97182900	-1.09403100	-0.67411500
Cl	-2.60295500	-0.95470500	0.00000000
H	-0.44524000	-1.82409000	0.00000000
H	2.78712100	-1.60819500	1.17164300
H	2.78712100	-1.60819500	-1.17164300

Table S3. Cartesian coordinates (in Å) of the structures optimized at the M05-2X/6-311++G** level.

radical				cation			
C -1.15334900	3.69935400	0.00000000		C 1.17796900	3.66119200	0.00000000	
C -1.54952200	2.37897400	0.00000000		C 1.56657500	2.35176800	0.00000000	
C -0.62516700	1.30800500	0.00000000		C 0.61553200	1.29021200	0.00000000	
C 0.75721800	1.63779100	0.00000000		C -0.77871000	1.61779100	0.00000000	
C 1.13146200	2.98595100	0.00000000		C -1.14017300	2.98025600	0.00000000	
C 0.20445200	4.01381700	0.00000000		C -0.19384100	3.97582800	0.00000000	
C -1.18679100	-0.00000200	0.00000000		C 1.16237200	0.00000000	0.00000000	
C 0.75721600	-1.63779200	0.00000000		C -0.77871000	-1.61779100	0.00000000	
C -0.62516400	-1.30801100	0.00000000		C 0.61553200	-1.29021200	0.00000000	
C -1.54953000	-2.37897200	0.00000000		C 1.56657500	-2.35176800	0.00000000	
H -2.60503800	-2.14090400	0.00000000		H 2.61861600	-2.10117100	0.00000000	
C -1.15334900	-3.69935000	0.00000000		C 1.17796900	-3.66119200	0.00000000	
C 0.20444900	-4.01381500	0.00000000		C -0.19384100	-3.97582800	0.00000000	
C 1.13146200	-2.98595200	0.00000000		C -1.14017300	-2.98025600	0.00000000	
H -1.89642400	4.48475000	0.00000000		H 1.91509200	4.45077300	0.00000000	
H -2.60503700	2.14091300	0.00000000		H 2.61861600	2.10117100	0.00000000	
H 2.18766900	3.22258000	0.00000000		H -2.19029800	3.23693700	0.00000000	
H 0.53265900	5.04351000	0.00000000		H -0.50630000	5.01099200	0.00000000	
H -1.89642300	-4.48475000	0.00000000		H 1.91509200	-4.45077300	0.00000000	
H 0.53265000	-5.04351000	0.00000000		H -0.50630000	-5.01099200	0.00000000	
H 2.18766900	-3.22258200	0.00000000		H -2.19029800	-3.23693700	0.00000000	
C 1.84341400	0.67149900	0.00000000		C -1.84994000	0.68063900	0.00000000	
C 1.84341200	-0.67149900	0.00000000		C -1.84994000	-0.68063900	0.00000000	
H -2.26916100	-0.00000100	0.00000000		H 2.24696700	0.00000000	0.00000000	
H 2.82508000	1.13117700	0.00000000		H -2.83218200	1.13687200	0.00000000	
H 2.82507600	-1.13118000	0.00000000		H -2.83218200	-1.13687200	0.00000000	
HBCIP				HBCIP (with BSSE)			
C 0.00000000	3.64529700	0.56322000		C 0.00000000	3.64528000	0.56248600	
C 0.00000000	2.32723700	0.94396000		C 0.00000000	2.32729500	0.94322600	
C 0.00000000	1.28963800	-0.02894400		C 0.00000000	1.28945700	-0.02933300	
C 0.00000000	1.62177300	-1.41634200		C 0.00000000	1.62162400	-1.41675200	
C 0.00000000	2.98312200	-1.76476200		C 0.00000000	2.98298400	-1.76530100	
C 0.00000000	3.96908600	-0.80099000		C 0.00000000	3.96912900	-0.80177300	
C 0.00000000	0.00000000	0.52825700		C 0.00000000	0.00000000	0.52822200	
C 0.00000000	-1.62177300	-1.41634200		C 0.00000000	-1.62162400	-1.41675200	
C 0.00000000	-1.28963800	-0.02894400		C 0.00000000	-1.28945700	-0.02933300	
C 0.00000000	-2.32723700	0.94396000		C 0.00000000	-2.32729500	0.94322600	
H 0.00000000	-2.03079200	1.99004500		H 0.00000000	-2.03181100	1.98930100	
C 0.00000000	-3.64529700	0.56322000		C 0.00000000	-3.64528000	0.56248600	
C 0.00000000	-3.96908600	-0.80099000		C 0.00000000	-3.96912900	-0.80177300	
C 0.00000000	-2.98312200	-1.76476200		C 0.00000000	-2.98298400	-1.76530100	
H 0.00000000	4.42695600	1.30881200		H 0.00000000	4.42689100	1.30814600	
H 0.00000000	2.03079200	1.99004500		H 0.00000000	2.03181100	1.98930100	
H 0.00000000	3.25358300	-2.81191200		H 0.00000000	3.25345000	-2.81248000	
H 0.00000000	5.00723900	-1.10534600		H 0.00000000	5.00725300	-1.10624000	
H 0.00000000	-4.42695600	1.30881200		H 0.00000000	-4.42689100	1.30814600	
H 0.00000000	-5.00723900	-1.10534600		H 0.00000000	-5.00725300	-1.10624000	
H 0.00000000	-3.25358300	-2.81191200		H 0.00000000	-3.25345000	-2.81248000	
C 0.00000000	0.67827100	-2.49295500		C 0.00000000	0.67826800	-2.49352400	

C 0.00000000 -0.67827100 -2.49295500	C 0.00000000 -0.67826800 -2.49352400
Cl 0.00000000 0.00000000 3.72635100	Cl 0.00000000 0.00000000 3.72969200
H 0.00000000 0.00000000 1.63015300	H 0.00000000 0.00000000 1.63040700
H 0.00000000 1.13723500 -3.47455600	H 0.00000000 1.13718500 -3.47514600
H 0.00000000 -1.13723500 -3.47455600	H 0.00000000 -1.13718500 -3.47514600
TS1	TS1 (with BSSE)
C 0.59092900 -0.25990000 3.65369400	C -0.58995200 -0.26701800 -3.65386700
C 0.96012000 -0.38612500 2.33878800	C -0.95901100 -0.39310700 -2.33893900
C 0.00971300 -0.24230400 1.29297100	C -0.00938000 -0.24510500 -1.29303500
C -1.34413700 0.05613500 1.61873300	C 1.34351200 0.05776600 -1.61878500
C -1.68809600 0.16213600 2.97830300	C 1.68741100 0.16372200 -2.97839200
C -0.74742700 0.00897300 3.97243900	C 0.74754100 0.00628900 -3.97258800
C 0.54711100 -0.42069300 0.00000000	C -0.54690400 -0.42228900 0.00000000
C -1.34413700 0.05613500 -1.61873300	C 1.34351200 0.05776600 1.61878500
C 0.00971300 -0.24230400 -1.29297100	C -0.00938000 -0.24510500 1.29303500
C 0.96012000 -0.38612500 -2.33878800	C -0.95901100 -0.39310700 2.33893900
H 1.99526800 -0.53547700 -2.05490200	H -1.99376400 -0.54560500 2.05539200
C 0.59092900 -0.25990000 -3.65369400	C -0.58995200 -0.26701800 3.65386700
C -0.74742700 0.00897300 -3.97243900	C 0.74754100 0.00628900 3.97258800
C -1.68809600 0.16213600 -2.97830300	C 1.68741100 0.16372200 2.97839200
H 1.32964700 -0.35516100 4.43625200	H -1.32817500 -0.36563500 -4.43647000
H 1.99526800 -0.53547700 2.05490200	H -1.99376400 -0.54560500 -2.05539200
H -2.71544000 0.37790900 3.23815500	H 2.71401500 0.38303100 -3.23821600
H -1.04473000 0.10885100 5.00742500	H 1.04466500 0.10640000 -5.00760000
H 1.32964700 -0.35516100 -4.43625200	H -1.32817500 -0.36563500 4.43647000
H -1.04473000 0.10885100 -5.00742500	H 1.04466500 0.10640000 5.00760000
H -2.71544000 0.37790900 -3.23815500	H 2.71401500 0.38303100 3.23821600
C -2.40859500 0.24113600 0.67689600	C 2.40705500 0.24751400 -0.67691000
C -2.40859500 0.24113600 -0.67689600	C 2.40705500 0.24751400 0.67691000
Cl 3.42789800 0.48554300 0.00000000	Cl -3.42765700 0.49408400 0.00000000
H 1.58838600 -0.72524300 0.00000000	H -1.58827700 -0.72599900 0.00000000
H -3.37244300 0.42116100 1.13809500	H 3.37014400 0.43160600 -1.13806400
H -3.37244300 0.42116100 -1.13809500	H 3.37014400 0.43160600 1.13806400
TS2	cov1
C -3.75898700 0.66230700 -0.09411600	C 0.69050500 -1.30576800 3.40399100
C -2.46279700 1.10308500 0.11661800	C 1.22092500 -0.91366200 2.18480100
C -1.35961400 0.24020500 0.16116500	C 0.46377300 -0.18751700 1.26727600
C -1.62195700 -1.13639000 0.03960000	C -0.86403300 0.14464800 1.57412100
C -2.94235200 -1.56429700 -0.18169700	C -1.37388800 -0.23132700 2.82271700
C -4.00645400 -0.69071500 -0.26339800	C -0.61509800 -0.95380400 3.72736000
C 0.00000000 0.87087200 0.50639000	C 1.12910000 0.25709400 0.00000000
C 1.62195700 -1.13639000 0.03960000	C -0.86403300 0.14464800 -1.57412100
C 1.35961400 0.24020500 0.16116500	C 0.46377300 -0.18751700 -1.26727600
C 2.46279700 1.10308500 0.11661800	C 1.22092500 -0.91366200 -2.18480100
H 2.31228800 2.16022200 0.25042000	H 2.24741700 -1.15805200 -1.94295700
C 3.75898700 0.66230700 -0.09411600	C 0.69050500 -1.30576800 -3.40399100
C 4.00645400 -0.69071500 -0.26339800	C -0.61509800 -0.95380400 -3.72736000
C 2.94235200 -1.56429700 -0.18169700	C -1.37388800 -0.23132700 -2.82271700
H -4.56584600 1.38107000 -0.12132100	H 1.29625600 -1.86471700 4.10332500
H -2.31228800 2.16022200 0.25042000	H 2.24741700 -1.15805200 1.94295700
H -3.11791500 -2.62643600 -0.28698600	H -2.39174100 0.04135000 3.07011600

H -5.00736900	-1.05919300	-0.43854000	H -1.03714900	-1.23925300	4.68080700
H 4.56584600	1.38107000	-0.12132100	H 1.29625600	-1.86471700	-4.10332500
H 5.00736900	-1.05919300	-0.43854000	H -1.03714900	-1.23925300	-4.68080700
H 3.11791500	-2.62643600	-0.28698500	H -2.39174100	0.04135000	-3.07011600
C -0.66626700	-2.23046200	0.15874400	C -1.75960700	0.86127400	0.67007700
C 0.66626700	-2.23046200	0.15874400	C -1.75960700	0.86127400	-0.67007700
Cl 0.00000000	2.57688000	-0.18435700	H -2.57057900	1.38735200	1.16049200
H 0.00000000	1.06032000	1.57954900	H -2.57057900	1.38735200	-1.16049200
H -1.13459600	-3.20431900	0.23302100	H 2.14836900	-0.11441600	0.00000000
H 1.13459600	-3.20431900	0.23302100	Cl 1.34339400	2.07484500	0.00000000
cov2					
C -0.51222700	1.23694200	3.21692200			
C -1.05714100	0.68307200	2.06773400			
C -0.28478300	-0.12308800	1.23845200			
C 1.06410100	-0.35329600	1.54949600			
C 1.58606600	0.18150900	2.73266900			
C 0.81041000	0.97533700	3.55900700			
C -0.81428900	-0.80501800	0.00000000			
C 1.06410100	-0.35329600	-1.54949600			
C -0.28478300	-0.12308800	-1.23845200			
C -1.05714100	0.68307200	-2.06773400			
H -2.09487700	0.85568700	-1.82448300			
C -0.51222700	1.23694200	-3.21692200			
C 0.81041000	0.97533700	-3.55900700			
C 1.58606600	0.18150900	-2.73266900			
H -1.12684400	1.85589800	3.85597000			
H -2.09487700	0.85568700	1.82448300			
H 2.61971800	-0.01860200	2.98423900			
H 1.23238100	1.39003800	4.46380500			
H -1.12684400	1.85589800	-3.85597000			
H 1.23238100	1.39003800	-4.46380500			
H 2.61971800	-0.01860200	-2.98423900			
C 1.96365800	-1.10635000	0.67190000			
C 1.96365800	-1.10635000	-0.67190000			
H 2.77451100	-1.62512300	1.17093500			
H 2.77451100	-1.62512300	-1.17093500			
Cl -2.60657000	-0.95194900	0.00000000			
H -0.45338500	-1.83206700	0.00000000			

Table S4. Cartesian coordinates (in Å) of the structures optimized at the MP2/6-31++G** level.

HBCIP				HBCIP (with BSSE)			
C	0.57203500	0.03889500	3.65456100	C	-0.55740400	-0.03179900	3.65965100
C	0.95620200	0.03036300	2.32989300	C	-0.94530000	-0.01996200	2.33588300
C	-0.02567600	-0.01998000	1.28974800	C	0.03187200	0.02973500	1.29076500
C	-1.42709600	0.00508600	1.62694200	C	1.43427600	-0.00941700	1.62602100
C	-1.76983100	-0.00045000	3.00499600	C	1.78116700	-0.00323300	3.00322400
C	-0.80136200	0.03944800	3.99189000	C	0.81663000	-0.03947000	3.99369100
C	0.53525400	-0.00180300	0.00000000	C	-0.53017200	0.01447200	0.00000000
C	-1.42709600	0.00508600	-1.62694200	C	1.43427600	-0.00941700	-1.62602100
C	-0.02567600	-0.01998000	-1.28974800	C	0.03187200	0.02973500	-1.29076500
C	0.95620200	0.03036300	-2.32989300	C	-0.94530000	-0.01996200	-2.33588300
H	2.00128300	0.02697200	-2.02747700	H	-1.99295200	-0.01401200	-2.04277000
C	0.57203500	0.03889500	-3.65456100	C	-0.55740400	-0.03179900	-3.65965100
C	-0.80136200	0.03944800	-3.99189000	C	0.81663000	-0.03947000	-3.99369100
C	-1.76983100	-0.00045000	-3.00499600	C	1.78116700	-0.00323300	-3.00322400
H	1.32132400	0.06949000	4.43538600	H	-1.30542400	-0.06119200	4.44170300
H	2.00128300	0.02697200	2.02747700	H	-1.99295200	-0.01401200	2.04277000
H	-2.81871600	0.00130800	3.27890200	H	2.83110200	-0.00943000	3.27301100
H	-1.10011200	0.04400100	5.03339900	H	1.11860600	-0.04500900	5.03422500
H	1.32132400	0.06949000	-4.43538600	H	-1.30542400	-0.06119200	-4.44170300
H	-1.10011200	0.04400100	-5.03339900	H	1.11860600	-0.04500900	-5.03422500
H	-2.81871600	0.00130800	-3.27890200	H	2.83110200	-0.00943000	-3.27301100
C	-2.49505800	-0.04974600	0.69115900	C	2.50264100	0.04237200	0.69104000
C	-2.49505800	-0.04974600	-0.69115900	C	2.50264100	0.04237200	-0.69104000
Cl	3.71763900	-0.03770300	0.00000000	Cl	-3.77875500	0.02404200	0.00000000
H	1.63822800	0.00128100	0.00000000	H	-1.63224600	0.01608800	0.00000000
H	-3.48387800	-0.07821600	1.14069500	H	3.49142600	0.06447000	1.14084700
H	-3.48387800	-0.07821600	-1.14069500	H	3.49142600	0.06447000	-1.14084700
TS1				TS1 (with BSSE)			
C	0.62120400	-0.31142700	3.66522900	C	0.60807400	-0.36682800	3.66840600
C	0.98740300	-0.46569200	2.34512000	C	0.97274800	-0.52505200	2.34847600
C	0.03835200	-0.28744900	1.29245500	C	0.02769800	-0.33506100	1.29394900
C	-1.31424500	0.07783200	1.62086200	C	-1.30724100	0.09348900	1.62095300
C	-1.65218500	0.19236100	2.99688500	C	-1.64717000	0.20719500	2.99673600
C	-0.71715600	0.00009800	3.99584800	C	-0.71715500	-0.00137800	3.99668500
C	0.56317800	-0.52126400	0.00000000	C	0.55688000	-0.54930500	0.00000000
C	-1.31424500	0.07783200	-1.62086200	C	-1.30724100	0.09348900	-1.62095300
C	0.03835200	-0.28744900	-1.29245500	C	0.02769800	-0.33506100	-1.29394900
C	0.98740300	-0.46569200	-2.34512000	C	0.97274800	-0.52505200	-2.34847600
H	2.02186500	-0.61681300	-2.05767200	H	2.00059700	-0.72604500	-2.07002900
C	0.62120400	-0.31142700	-3.66522900	C	0.60807400	-0.36682800	-3.66840600
C	-0.71715600	0.00009800	-3.99584800	C	-0.71715500	-0.00137800	-3.99668500
C	-1.65218500	0.19236100	-2.99688500	C	-1.64717000	0.20719500	-2.99673600
H	1.36070800	-0.42608600	4.44756300	H	1.34464300	-0.49698400	4.45097200
H	2.02186500	-0.61681300	2.05767200	H	2.00059700	-0.72604500	2.07002900
H	-2.67281800	0.44900600	3.25690600	H	-2.65760400	0.50325300	3.25432400
H	-1.00836400	0.10939200	5.03359300	H	-1.00685400	0.11405300	5.03413200
H	1.36070800	-0.42608600	-4.44756300	H	1.34464300	-0.49698400	-4.45097200
H	-1.00836400	0.10939200	-5.03359300	H	-1.00685400	0.11405300	-5.03413200
H	-2.67281800	0.44900600	-3.25690600	H	-2.65760400	0.50325300	-3.25432400

C -2.37159000	0.27332800	0.68911900	C -2.35695700	0.32222100	0.68922200
C -2.37159000	0.27332800	-0.68911900	C -2.35695700	0.32222100	-0.68922200
Cl 3.24784900	0.60547400	0.00000000	Cl 3.25882100	0.68159100	0.00000000
H 1.57856200	-0.89878000	0.00000000	H 1.56692300	-0.93901300	0.00000000
H -3.33762000	0.47684200	1.14238300	H -3.31483900	0.56210700	1.14193600
H -3.33762000	0.47684200	-1.14238300	H -3.31483900	0.56210700	-1.14193600
TS2			cov1		
C -0.67397800	-0.04189600	3.77663600	C 0.68151400	-1.34149500	3.39113600
C -1.11176400	0.16159000	2.46903700	C 1.21807800	-0.93360600	2.17041400
C -0.24501800	0.15687900	1.35590700	C 0.46397100	-0.18067600	1.25670000
C 1.14186000	0.03514200	1.62516200	C -0.87189800	0.16064000	1.57065700
C 1.56333900	-0.19916500	2.95574800	C -1.38577900	-0.22887600	2.82513800
C 0.68323300	-0.24145100	4.02856200	C -0.62908600	-0.97756300	3.72324600
C -0.88087800	0.49874600	0.00000000	C 1.13554100	0.27770900	0.00000000
C 1.14186000	0.03514200	-1.62516200	C -0.87189800	0.16064000	-1.57065700
C -0.24501800	0.15687900	-1.35590700	C 0.46397100	-0.18067600	-1.25670000
C -1.11176400	0.16159000	-2.46903700	C 1.21807800	-0.93360600	-2.17041400
H -2.16837500	0.31192200	-2.31465100	H 2.24531600	-1.18140300	-1.92481500
C -0.67397800	-0.04189600	-3.77663600	C 0.68151400	-1.34149500	-3.39113600
C 0.68323300	-0.24145100	-4.02856200	C -0.62908600	-0.97756300	-3.72324600
C 1.56333900	-0.19916500	-2.95574800	C -1.38577900	-0.22887600	-2.82513800
H -1.39405200	-0.03104300	4.58564100	H 1.28341300	-1.91723400	4.08351700
H -2.16837500	0.31192200	2.31465100	H 2.24531600	-1.18140300	1.92481500
H 2.62546800	-0.32309100	3.13448700	H -2.40389700	0.04700000	3.07804900
H 1.04815100	-0.41834600	5.03271000	H -1.05395700	-1.27153800	4.67526500
H -1.39405200	-0.03104300	-4.58564100	H 1.28341300	-1.91723400	-4.08351700
H 1.04815100	-0.41834600	-5.03271000	H -1.05395700	-1.27153800	-4.67526500
H 2.62546800	-0.32309100	-3.13448700	H -2.40389700	0.04700000	-3.07804900
C 2.23831700	0.13838500	0.67505700	C -1.75476000	0.90124400	0.67944700
C 2.23831700	0.13838500	-0.67505700	C -1.75476000	0.90124400	-0.67944700
Cl -2.55494900	-0.24537600	0.00000000	H -2.55810400	1.44601300	1.16755000
H -1.08944400	1.57348900	0.00000000	H -2.55810400	1.44601300	-1.16755000
H 3.21729600	0.20636700	1.13961700	H 2.15068500	-0.11875500	0.00000000
H 3.21729600	0.20636700	-1.13961700	Cl 1.37329700	2.08298900	0.00000000
cov2					
C -0.50614700	1.28313200	3.18698500			
C -1.05905800	0.71015900	2.04100400			
C -0.29121000	-0.13025400	1.22516300			
C 1.06555200	-0.37104000	1.54452300			
C 1.59501100	0.18460100	2.72647300			
C 0.82141500	1.00874000	3.53984000			
C -0.82370200	-0.82747700	0.00000000			
C 1.06555200	-0.37104000	-1.54452300			
C -0.29121000	-0.13025400	-1.22516300			
C -1.05905800	0.71015900	-2.04100400			
H -2.09799100	0.88740800	-1.79646800			
C -0.50614700	1.28313200	-3.18698500			
C 0.82141500	1.00874000	-3.53984000			
C 1.59501100	0.18460100	-2.72647300			
H -1.11553600	1.92235800	3.81425000			
H -2.09799100	0.88740800	1.79646800			

H	2.62894300	-0.01833700	2.98430200
H	1.24698800	1.43632500	4.43943900
H	-1.11553600	1.92235800	-3.81425000
H	1.24698800	1.43632500	-4.43943900
H	2.62894300	-0.01833700	-2.98430200
C	1.94992100	-1.15045600	0.68118300
C	1.94992100	-1.15045600	-0.68118300
Cl	-2.60773200	-0.98028900	0.00000000
H	-0.45380400	-1.85625000	0.00000000
H	2.74842500	-1.69404200	1.17889500
H	2.74842500	-1.69404200	-1.17889500

Table S5. Cartesian coordinates (in Å) of the structures optimized at the MP2/6-311++G**(H,Cl)/6-31++G**(C) level.

HBCIP				HBCIP (with BSSE)			
C	-0.57331800	-0.03104400	3.65909800	C	-0.55900500	-0.02696900	3.66334500
C	-0.95824300	-0.03193700	2.33344100	C	-0.94689600	-0.02375200	2.33833600
C	0.02289900	0.01716100	1.29120800	C	0.02988300	0.02645300	1.29189700
C	1.42560100	-0.00832300	1.62844100	C	1.43342500	-0.01071500	1.62757600
C	1.76912500	0.00428500	3.00716300	C	1.78046200	0.00092300	3.00572900
C	0.80120900	-0.03734700	3.99594800	C	0.81599500	-0.03845800	3.99756200
C	-0.53770900	-0.01062800	0.00000000	C	-0.53177900	0.00256300	0.00000000
C	1.42560100	-0.00832300	-1.62844100	C	1.43342500	-0.01071500	-1.62757600
C	0.02289900	0.01716100	-1.29120800	C	0.02988300	0.02645300	-1.29189700
C	-0.95824300	-0.03193700	-2.33344100	C	-0.94689600	-0.02375200	-2.33833600
H	-2.00647800	-0.02691200	-2.03072300	H	-1.99737700	-0.01725000	-2.04431300
C	-0.57331800	-0.03104400	-3.65909800	C	-0.55900500	-0.02696900	-3.66334500
C	0.80120900	-0.03734700	-3.99594800	C	0.81599500	-0.03845800	-3.99756200
C	1.76912500	0.00428500	-3.00716300	C	1.78046200	0.00092300	-3.00572900
H	-1.32500100	-0.05973200	4.44219900	H	-1.30974100	-0.05532500	4.44735900
H	-2.00647800	-0.02691200	2.03072300	H	-1.99737700	-0.01725000	2.04431300
H	2.82156000	0.00070700	3.28020600	H	2.83380500	-0.00653200	3.27508400
H	1.10214500	-0.03808600	5.04025300	H	1.11974900	-0.04139800	5.04100800
H	-1.32500100	-0.05973200	-4.44219900	H	-1.30974100	-0.05532500	-4.44735900
H	1.10214500	-0.03808600	-5.04025300	H	1.11974900	-0.04139800	-5.04100800
H	2.82156000	0.00070700	-3.28020600	H	2.83380500	-0.00653200	-3.27508400
C	2.49352000	0.04808400	0.69161800	C	2.50175900	0.04247900	0.69157100
C	2.49352000	0.04808400	-0.69161800	C	2.50175900	0.04247900	-0.69157100
Cl	-3.70893000	0.03788900	0.00000000	Cl	-3.77167900	0.02679000	0.00000000
H	-1.64690000	-0.01490900	0.00000000	H	-1.63858300	0.00177300	0.00000000
H	3.48550000	0.07602900	1.14196400	H	3.49372300	0.06444900	1.14212300
H	3.48550000	0.07602900	-1.14196400	H	3.49372300	0.06444900	-1.14212300
TS1				TS1 (with BSSE)			
C	0.61980400	-0.29148100	3.66681900	C	0.60354200	-0.36251000	3.67126800
C	0.98620900	-0.44625400	2.34557900	C	0.96996400	-0.51395100	2.34980800
C	0.02974500	-0.29303400	1.29397000	C	0.02142600	-0.33334800	1.29537100
C	-1.32262500	0.07913900	1.62243000	C	-1.31496000	0.09505800	1.62291700
C	-1.66209400	0.18523100	2.99951200	C	-1.65641700	0.20175400	2.99964100
C	-0.72053800	0.01591700	3.99814000	C	-0.72271500	0.00334300	3.99981400
C	0.56074200	-0.50351800	0.00000000	C	0.55569200	-0.52703800	0.00000000
C	-1.32262500	0.07913900	-1.62243000	C	-1.31496000	0.09505800	-1.62291700
C	0.02974500	-0.29303400	-1.29397000	C	0.02142600	-0.33334800	-1.29537100
C	0.98620900	-0.44625400	-2.34557900	C	0.96996400	-0.51395100	-2.34980800
H	2.02346300	-0.59682400	-2.05511900	H	2.00026700	-0.71718900	-2.06915700
C	0.61980400	-0.29148100	-3.66681900	C	0.60354200	-0.36251000	-3.67126800
C	-0.72053800	0.01591700	-3.99814000	C	-0.72271500	0.00334300	-3.99981400
C	-1.66209400	0.18523100	-2.99951200	C	-1.65641700	0.20175400	-2.99964100
H	1.36511100	-0.39104100	4.45026000	H	1.34364600	-0.48871900	4.45567800
H	2.02346300	-0.59682400	2.05511900	H	2.00026700	-0.71718900	2.06915700
H	-2.68663700	0.43936700	3.26013300	H	-2.67036700	0.49724500	3.25760400
H	-1.01251000	0.12556900	5.03908100	H	-1.01412000	0.11676300	5.04044700
H	1.36511100	-0.39104100	-4.45026000	H	1.34364600	-0.48871900	-4.45567800

H -1.01251000	0.12556900	-5.03908100	H -1.01412000	0.11676300	-5.04044700
H -2.68663700	0.43936700	-3.26013300	H -2.67036700	0.49724500	-3.25760400
C -2.38336600	0.25470000	0.68982500	C -2.36594600	0.31559100	0.68991800
C -2.38336600	0.25470000	-0.68982500	C -2.36594600	0.31559100	-0.68991800
Cl 3.28317000	0.57534700	0.00000000	Cl 3.29457700	0.66284200	0.00000000
H 1.58604000	-0.86530100	0.00000000	H 1.57619100	-0.89975200	0.00000000
H -3.35443100	0.45036900	1.14363700	H -3.32786200	0.55311000	1.14311100
H -3.35443100	0.45036900	-1.14363700	H -3.32786200	0.55311000	-1.14311100
TS2			cov1		
C -3.77749700	0.67441100	-0.05466100	C 0.70718900	-1.33220500	3.39252400
C -2.46989200	1.11244700	0.15552500	C 1.23728600	-0.91430300	2.17113000
C -1.35580600	0.24548200	0.15801500	C 0.46972700	-0.17320900	1.25758300
C -1.62532500	-1.14256400	0.03648700	C -0.87290400	0.14536300	1.57171700
C -2.95561000	-1.56471500	-0.20289300	C -1.37971800	-0.25229000	2.82750500
C -4.02931300	-0.68431100	-0.25167000	C -0.61010100	-0.98976500	3.72554600
C 0.00000000	0.87954100	0.50352700	C 1.13055500	0.29827100	0.00000000
C 1.62531900	-1.14256600	0.03646500	C -0.87290400	0.14536300	-1.57171700
C 1.35580600	0.24547800	0.15802400	C 0.46972700	-0.17320900	-1.25758300
C 2.46989600	1.11243700	0.15556200	C 1.23728600	-0.91430300	-2.17113000
H 2.31602500	2.17209600	0.30654600	H 2.27147600	-1.14515700	-1.92371600
C 3.77749900	0.67440100	-0.05463300	C 0.70718900	-1.33220500	-3.39252400
C 4.02930800	-0.68431600	-0.25168500	C -0.61010100	-0.98976500	-3.72554600
C 2.95560200	-1.56471700	-0.20292900	C -1.37971800	-0.25229000	-2.82750500
H -4.58848500	1.39722700	-0.04832800	H 1.32057500	-1.89975900	4.08671500
H -2.31601700	2.17210800	0.30647900	H 2.27147600	-1.14515700	1.92371600
H -3.13342500	-2.63062900	-0.32362300	H -2.40538400	0.00720800	3.08107700
H -5.03563300	-1.05097700	-0.43261800	H -1.03106600	-1.29173400	4.68057100
H 4.58849100	1.39721200	-0.04827700	H 1.32057500	-1.89975900	-4.08671500
H 5.03562600	-1.05098100	-0.43264500	H -1.03106600	-1.29173400	-4.68057100
H 3.13341200	-2.63062900	-0.32368500	H -2.40538400	0.00720800	-3.08107700
C -0.67555600	-2.23886000	0.15119300	C -1.76703200	0.87283300	0.67993700
C 0.67554900	-2.23886100	0.15117800	C -1.76703200	0.87283300	-0.67993700
Cl 0.00000800	2.55779000	-0.23309800	Cl 1.32350000	2.10929200	0.00000000
H -0.00000400	1.08284000	1.58130400	H 2.15582300	-0.07762000	0.00000000
H -1.14141200	-3.22021200	0.22625000	H -2.58160800	1.40591100	1.16914300
H 1.14140600	-3.22021400	0.22622400	H -2.58160800	1.40591100	-1.16914300
cov2					
C -0.50816800	1.28262100	3.19266000			
C -1.06055800	0.71115900	2.04445900			
C -0.29078600	-0.12632400	1.22547000			
C 1.06620500	-0.36987800	1.54717100			
C 1.59430100	0.18277500	2.73241300			
C 0.81912800	1.00485200	3.54810400			
C -0.82256500	-0.82327200	0.00000000			
C 1.06620500	-0.36987800	-1.54717100			
C -0.29078600	-0.12632400	-1.22547000			
C -1.06055800	0.71115900	-2.04445900			
H -2.10168000	0.89132100	-1.79746800			
C -0.50816800	1.28262100	-3.19266000			
C 0.81912800	1.00485200	-3.54810400			
C 1.59430100	0.18277500	-2.73241300			

H	-1.12014300	1.92208600	3.82279800
H	-2.10168000	0.89132100	1.79746800
H	2.63081000	-0.02253400	2.99155200
H	1.24496700	1.43097600	4.45221700
H	-1.12014300	1.92208600	-3.82279800
H	1.24496700	1.43097600	-4.45221700
H	2.63081000	-0.02253400	-2.99155200
C	1.95176900	-1.14603800	0.68174000
C	1.95176900	-1.14603800	-0.68174000
Cl	-2.60601700	-0.98525800	0.00000000
H	-0.44571400	-1.85139900	0.00000000
H	2.75639900	-1.68664600	1.17953400
H	2.75639900	-1.68664600	-1.17953400

Table S6. Vibrational frequencies (in cm⁻¹) computed at the M05-2X/6-31++G** level.

radical(C _{2v})	cation(C _s ~C _{2v})	HBCIP(C _{2v})	TS1(C _s)	cov1(C _s)	cov2(C _s)	TS2(C _s)
47.7717(B ₁)	65.5887(A'')	44.9946(B ₁) ^a	-59.6432(A')	51.8622(A')	56.6282(A')	-66.4998(A')
95.4877(A ₂)	88.7111(A'')	(41.8727) ^b	(-63.9940) ^b	96.2128(A'')	93.7283(A'')	68.3900(A'')
195.5252(B ₁)	194.8278(A'')	62.8452(B ₂) ^a	55.3993(A')	112.5069(A')	129.1651(A')	88.5957(A')
202.9800(A ₂)	195.5410(A'')	(58.7435)	(55.3430)	124.4372(A'')	176.1979(A'')	194.3545(A'')
240.9864(A ₁)	242.2429(A')	68.7763(B ₁) ^a	70.7494(A'')	180.8635(A')	188.5523(A')	207.1920(A')
294.3761(B ₁)	335.2496(A'')	(66.0914)	(70.1315)	245.1908(A'')	229.6144(A'')	251.8019(A')
335.3259(B ₂)	337.0406(A')	98.6448(A ₂)	97.5537(A'')	272.5288(A')	262.1372(A')	292.0750(A'')
338.0725(A ₁)	347.5401(A')	(97.1540)	(96.0051)	323.8270(A')	318.1396(A')	293.5011(A')
395.6724(A ₂)	383.2153(A'')	163.1099(A ₁) ^a	143.4862(A')	325.0925(A'')	321.4410(A'')	332.6306(A'')
440.5251(B ₁)	434.0089(A'')	(157.6420)	(144.4085)	343.7543(A')	394.7154(A'')	366.1008(A')
499.3383(A ₂)	478.1359(A'')	193.4882(A ₂)	192.1907(A'')	398.2459(A'')	411.9050(A')	394.9139(A'')
505.2434(B ₂)	503.1880(A'')	(193.0145)	(192.0639)	465.9881(A')	462.4209(A')	436.8760(A')
526.3445(A ₁)	525.6491(A'')	197.0145(B ₁)	207.9556(A')	480.7043(A'')	470.6614(A'')	485.8767(A')
547.7585(B ₁)	543.4351(A'')	(197.1935)	(207.9302)	529.6513(A')	490.6302(A')	490.7315(A'')
587.8557(A ₂)	564.9206(A'')	252.5532(A ₁) ^a	236.1972(A')	531.5449(A'')	518.3593(A'')	525.4280(A'')
622.7392(B ₂)	616.9781(A'')	(250.4458)	(236.1924)	543.3597(A')	555.5267(A')	548.5745(A')
661.8649(A ₁)	659.7074(A')	328.4844(B ₁)	335.5306(A'')	595.7966(A'')	597.3609(A'')	594.1198(A'')
715.9806(B ₁)	723.5803(A'')	(326.4670)	(335.4236)	627.3194(A'')	611.5107(A'')	629.8460(A'')
723.5680(A ₁)	725.9345(A'')	339.7483(B ₂)	339.6807(A')	650.4677(A')	641.1319(A')	644.4438(A')
736.4612(B ₂)	735.4325(A'')	(339.4799)	(339.4067)	720.6036(A')	714.7172(A'')	681.1821(A')
749.0170(B ₁)	767.2818(A'')	350.4850(A ₁) ^a	372.6533(A')	722.4793(A'')	726.4836(A')	737.3739(A'')
767.2010(A ₂)	778.0701(A'')	(349.7380)	(371.6554)	734.6123(A')	754.7820(A')	739.4580(A')
779.1798(A ₂)	798.5334(A'')	387.8499(A ₂)	387.5622(A'')	750.1205(A')	762.4491(A'')	745.3389(A')
819.4934(B ₁)	840.7330(A')	(386.7168)	(387.1996)	770.1901(A'')	791.7348(A'')	765.0279(A'')
838.5373(B ₁)	863.2758(A'')	440.7200(B ₁)	445.1888(A')	788.8927(A'')	793.2407(A')	791.2594(A'')
843.6736(B ₂)	880.8890(A')	(439.3693)	(443.4725)	812.5677(A')	818.9724(A')	808.1734(A')
871.3962(A ₁)	910.3485(A')	482.3812(A ₂)	479.3275(A'')	831.0208(A')	832.3251(A')	831.7345(A')
893.8807(A ₂)	927.2206(A'')	(482.0662)	(479.0848)	851.8022(A'')	855.2585(A')	850.0251(A'')
909.1094(B ₁)	944.2720(A')	504.0344(B ₂)	504.7242(A'')	871.6635(A')	889.3366(A')	854.0762(A')
939.7510(B ₂)	995.5917(A'')	(503.9704)	(504.5135)	909.4632(A'')	898.0974(A'')	903.7477(A'')
978.8633(A ₂)	1017.5527(A'')	525.2728(A ₁)	520.2334(A')	919.1077(A')	913.2525(A'')	920.2222(A')
984.0856(B ₁)	1031.0114(A'')	(524.8580)	(520.2303)	925.8423(A'')	922.7313(A')	920.5694(A'')
1012.6518(A ₂)	1047.5487(A'')	544.2826(B ₁)	550.0703(A')	987.9177(A'')	989.8727(A'')	996.2771(A'')
1014.2379(B ₁)	1050.9576(A'')	(544.3462)	(549.2532)	990.8153(A')	993.5652(A')	1000.7042(A')
1034.0657(A ₂)	1057.3979(A'')	575.0236(A ₂)	574.0528(A'')	1020.5353(A'')	1022.2673(A'')	1023.0727(A'')
1089.2791(A ₁)	1078.4585(A')	(574.0712)	(573.6034)	1024.1106(A')	1025.2096(A')	1025.7716(A')
1097.2100(B ₂)	1087.7534(A')	615.0778(B ₂)	616.5522(A'')	1029.1819(A'')	1028.4606(A'')	1035.6634(A'')
1156.0817(B ₂)	1172.8036(A')	(615.1198)	(616.5011)	1093.0069(A')	1090.3052(A')	1107.9436(A')
1159.2117(A ₁)	1175.5414(A')	660.3193(A ₁)	657.5719(A')	1097.7157(A'')	1092.5965(A'')	1121.3377(A'')
1181.2408(B ₂)	1212.3233(A')	(659.4317)	(657.4764)	1145.1827(A')	1127.2250(A')	1142.7525(A')
1192.4314(A ₁)	1214.9432(A')	727.4849(B ₁)	721.5253(A')	1154.7571(A'')	1138.6435(A'')	1152.9845(A'')
1204.6639(A ₁)	1225.1935(A')	(729.5276)	(722.2369)	1195.3252(A')	1197.8873(A')	1190.6130(A')
1212.8568(B ₂)	1237.1742(A')	731.6614(A ₁)	729.1160(A')	1197.2613(A'')	1200.1930(A'')	1200.6139(A')
1229.9418(A ₁)	1246.6252(A')	(730.3392)	(729.0960)	1203.2857(A')	1202.4300(A')	1208.3565(A'')
1272.4249(B ₂)	1284.3326(A')	734.5295(B ₂)	735.0010(A'')	1234.8826(A')	1221.2184(A'')	1223.0193(A')
1281.8466(A ₁)	1307.1372(A')	(734.4981)	(734.9603)	1242.3723(A'')	1242.8050(A')	1236.5802(A'')
1329.8873(B ₂)	1370.5677(A')	775.5967(A ₂)	764.6872(A')	1256.9514(A'')	1262.1838(A'')	1239.9998(A')
1345.2396(A ₁)	1380.7115(A')	(773.9882)	(765.2287)	1270.2778(A')	1263.5834(A')	1251.2309(A'')
1391.2991(A ₁)	1453.1861(A')	783.9721(B ₁)	770.0385(A'')	1281.4142(A')	1312.5784(A')	1288.3342(A')

1394.3842(B ₂)	1460.5649(A')	(784.2942)	(770.2541)	1292.7870(A'')	1320.4591(A'')	1300.4150(A'')
1453.5070(B ₂)	1473.2665(A')	805.8184(A ₂)	795.3693(A'')	1342.2218(A')	1335.6042(A'')	1350.1726(A'')
1461.3080(B ₂)	1485.5519(A')	(805.5245)	(795.6575)	1377.4773(A'')	1347.1313(A')	1350.3537(A')
1481.6164(A ₁)	1527.9027(A')	848.4194(B ₂)	849.9545(A')	1385.7861(A')	1376.1584(A'')	1375.3881(A'')
1510.4051(B ₂)	1542.4813(A')	(848.1502)	(850.3513)	1410.9540(A'')	1379.9534(A')	1397.3044(A')
1537.1728(A ₁)	1560.6016(A')	866.9440(B ₁)	851.4625(A'')	1468.4444(A'')	1455.9167(A'')	1477.1496(A'')
1558.4379(B ₂)	1590.6361(A')	(866.8677)	(851.1461)	1500.1319(A')	1503.8374(A')	1491.3567(A')
1630.2188(A ₁)	1602.1592(A')	879.4693(A ₁)	876.2967(A')	1527.1379(A'')	1521.4773(A'')	1520.0760(A'')
1639.6939(B ₂)	1643.4566(A')	(878.6404)	(876.2206)	1557.7838(A')	1548.9329(A')	1566.6140(A')
1677.6866(B ₂)	1690.7199(A')	925.2114(A ₂)	885.2867(A')	1569.4913(A'')	1554.8353(A'')	1567.1017(A'')
1681.2119(A ₁)	1697.8671(A')	(924.7231)	(884.6373)	1663.3407(A')	1658.0926(A')	1674.6020(A'')
1726.2512(A ₁)	1702.4403(A')	933.0445(B ₁)	911.9360(A'')	1675.5589(A'')	1670.0615(A'')	1678.0190(A')
3176.6126(B ₂)	3200.4279(A')	(933.2394)	(912.0824)	1705.2778(A')	1698.7458(A')	1701.6590(A')
3197.2053(A ₁)	3204.2152(A')	946.7577(B ₂)	932.4436(A')	1708.5112(A'')	1702.1281(A'')	1701.8371(A'')
3202.3503(A ₁)	3218.9681(A')	(946.7186)	(932.8370)	1731.5248(A')	1718.3198(A')	1767.3666(A')
3219.4504(B ₂)	3244.6048(A')	1031.8514(A ₂)	944.8312(A'')	3166.6477(A')	3137.4024(A')	3110.6710(A')
3220.2188(A ₁)	3244.8121(A')	(1031.7662)	(944.7712)	3220.0550(A'')	3222.1422(A'')	3203.2317(A'')
3232.6840(B ₂)	3262.0959(A')	1032.5450(B ₁)	1017.7081(A'')	3223.4337(A')	3232.9746(A')	3220.2871(A')
3233.0124(A ₁)	3263.0932(A')	(1032.1572)	(1018.1861)	3223.5199(A'')	3233.3836(A'')	3224.8105(A'')
3239.3102(B ₂)	3264.0955(A')	1047.4319(A ₂)	1024.4295(A')	3235.0663(A')	3241.3075(A')	3227.4927(A')
3240.4726(A ₁)	3264.1792(A')	(1047.6031)	(1024.5893)	3235.3540(A'')	3251.3615(A'')	3232.3756(A'')
3260.4764(B ₂)	3278.5743(A')	1056.4531(B ₁)	1040.0196(A'')	3239.4009(A')	3251.4812(A')	3233.1278(A')
3260.5517(A ₁)	3278.8250(A')	(1054.8538)	(1040.1643)	3244.3147(A'')	3259.2334(A'')	3250.8189(A'')
		1068.2818(A ₂)	1043.3864(A')	3244.9978(A')	3259.5421(A')	3250.9582(A')
		(1066.4076)	(1043.5559)	3251.1996(A'')	3273.7129(A'')	3290.7352(A'')
		1082.3470(A ₁)	1049.6988(A'')	3251.6032(A')	3273.9162(A')	3291.8771(A')
		(1082.2406)	(1048.8876)			
		1092.9925(B ₂)	1082.7683(A')			
		(1092.8641)	(1082.8137)			
		1119.6877(B ₁)	1093.8754(A'')			
		(1116.1273)	(1093.9927)			
		1164.8981(A ₁)	1166.4255(A'')			
		(1164.7160)	(1166.6210)			
		1165.5873(B ₂)	1167.8496(A')			
		(1165.4961)	(1167.9800)			
		1202.1637 (A ₁)	1202.6106(A')			
		(1202.0602)	(1202.7401)			
		1211.3258(B ₂)	1209.3173(A'')			
		(1211.2217)	(1209.5110)			
		1224.1455(A ₁)	1224.2281(A')			
		(1223.7090)	(1224.3343)			
		1242.6813(A ₁)	1238.5386(A')			
		(1242.4661)	(1238.6955)			
		1256.5976(B ₂)	1251.6914(A'')			
		(1255.9164)	(1251.3389)			
		1293.0022(B ₂)	1288.2353(A'')			
		(1292.3505)	(1288.1150)			
		1315.4933(A ₁)	1306.8198(A')			
		(1314.7714)	(1307.1985)			
		1359.6813(A ₁)	1358.5956(A')			
		(1359.2438)	(1358.7010)			
		1393.1648(B ₂)	1379.9087(A'')			
		(1392.8913)	(1379.5653)			

	1431.3415(A ₁) (1431.2476)	1428.5703(A') (1428.7810)		
	1461.4890(B ₂) (1461.1637)	1451.6793(A'') (1451.7003)		
	1474.2523(B ₂) (1473.8745)	1468.8434(A'') (1468.5350)		
	1485.7444 (A ₁) (1485.5926)	1485.3419(A') (1485.4514)		
	1539.0893(B ₂) (1538.4473)	1532.9362(A'') (1532.5821)		
	1544.3544(A ₁) (1543.9809)	1541.4920(A') (1541.5862)		
	1572.7395(B ₂) (1572.3378)	1566.3171(A'') (1566.5932)		
	1597.6425(A ₁) (1597.6463)	1605.5651(A') (1605.4123)		
	1629.5124(B ₂) (1629.5143)	1610.0370(A'') (1609.5464)		
	1660.8791(B ₂) (1660.2316)	1644.2253(A'') (1643.5984)		
	1695.0159(A ₁) (1695.0344)	1696.1664(A') (1696.1772)		
	1695.4155(B ₂) (1695.3276)	1696.3567(A'') (1696.3411)		
	1701.6868(A ₁) (1701.7618)	1706.9550(A') (1706.8353)		
	2941.0051(A ₁) ^c (2927.1595)	3206.2395(A') (3206.4089)		
	3190.0459(B ₂) (3190.2347)	3212.4112(A'') (3211.8684)		
	3207.5025(A ₁) (3207.6355)	3221.0354(A'') (3220.9727)		
	3210.5831(B ₂) (3211.4967)	3224.1356(A') (3224.1597)		
	3215.1014(A ₁) (3215.9211)	3229.5813(A') (3229.1124)		
	3241.3344(B ₂) (3241.4907)	3232.1340(A'') (3232.2692)		
	3241.5287(A ₁) (3241.6907)	3232.6446(A') (3232.6980)		
	3251.9179(B ₂) (3252.0578)	3258.1521(A'') (3258.2422)		
	3251.9702(A ₁) (3252.1063)	3258.2773(A') (3258.3632)		
	3267.3354(B ₂) (3267.3815)	3276.9293(A'') (3277.3363)		
	3267.3817(A ₁) (3267.4304)	3276.9804(A') (3277.3877)		

^aIntermolecular modes; ^bValues in parenthesis have been obtained with BSSE; ^cVery intense C–H stretching mode characteristic of the C⁺–H•••Cl[−] hydrogen bond.

Table S7. Vibrational frequencies (in cm^{-1}) computed at the M05-2X/6-311++G**(H,Cl)/6-31++G**(C) level.

HBCIP(C_{2v})	TS1(C_s)	cov1(C_s)	cov2(C_s)	TS2(C_s)
44.0115(B_1) ^a	-68.3815(A')	52.0577(A')	57.0452(A')	-69.5921(A')
(40.1050) ^b	(-62.6853)	96.5320(A'')	94.7177(A'')	65.7678(A'')
64.6498(B_2) ^a	55.8964(A')	112.4101(A')	129.5912(A')	87.7587(A')
(59.4761)	(56.6844)	125.2771(A'')	177.5042(A'')	194.5916(A'')
71.6218(B_1) ^a	70.0502(A'')	181.5883(A')	190.6109(A')	207.8512(A')
(66.5621)	(70.1687)	245.8135(A'')	231.8752(A'')	251.7925(A')
98.3622(A_2)	99.3148(A'')	273.2553(A')	263.6818(A')	292.1997(A'')
(97.3212)	(97.7553)	324.3534(A')	318.8703(A')	293.5687(A')
164.0895(A_1) ^a	145.8160(A')	325.7548(A'')	321.3626(A'')	332.4308(A'')
(157.0172)	(146.4314)	344.7744(A')	396.2810(A'')	366.4205(A')
194.3428(A_2)	194.7665(A'')	399.1017(A'')	412.4484(A')	396.0305(A'')
(194.1055)	(194.7606)	466.8441(A')	463.4136(A')	437.2756(A')
197.9666(B_1)	209.7074(A')	481.2334(A'')	471.7004(A'')	486.9983(A')
(197.8900)	(209.7993)	530.5529(A')	491.6562(A')	490.7506(A'')
252.7259(A_1) ^a	236.0504(A')	532.2206(A'')	518.5390(A'')	525.4910(A'')
(250.2431)	(236.4019)	544.3910(A')	556.0421(A')	548.5600(A')
335.3539(B_1)	336.0046(A'')	596.3451(A'')	598.0553(A'')	595.1620(A'')
(333.1566)	(335.9052)	627.4545(A'')	611.5951(A'')	629.9276(A'')
339.3928(B_2)	338.9504(A')	651.7382(A')	641.7332(A')	644.9054(A')
(339.2007)	(340.1060)	722.5474(A')	715.8303(A'')	681.6836(A')
350.7849(A_1) ^a	368.2983(A')	723.1485(A')	728.3053(A')	738.0479(A'')
(349.8417)	(370.4401)	736.0400(A')	757.2496(A')	739.5729(A')
390.7268(A_2)	392.3747(A'')	751.6430(A')	764.8965(A'')	745.8791(A')
(390.2041)	(392.1891)	772.2028(A')	794.3206(A')	765.7519(A'')
442.2870(B_1)	441.1835(A')	789.7622(A')	794.3384(A'')	791.0187(A'')
(440.5054)	(442.9621)	815.1417(A')	821.1842(A')	808.2655(A')
485.0609(A_2)	483.8196(A'')	833.8151(A')	835.7164(A')	832.9557(A')
(485.1151)	(483.5866)	853.8636(A'')	857.2564(A'')	850.4482(A'')
503.8738(B_2)	504.6056(A'')	873.0220(A')	890.6022(A')	854.3676(A')
(503.7287)	(504.5031)	911.8371(A'')	900.4070(A'')	903.9651(A'')
525.5622(A_1)	520.4802(A')	921.8082(A')	914.8496(A'')	920.5794(A')
(525.0666)	(520.8869)	926.7956(A'')	925.6518(A')	921.0735(A'')
549.5767(B_1)	547.2046(A')	991.6456(A'')	995.0789(A'')	998.4923(A'')
(548.8775)	(550.1406)	994.5790(A')	998.6934(A')	1002.3966(A')
578.0988(A_2)	578.6302(A'')	1022.9745(A'')	1026.4791(A'')	1024.2202(A'')
(577.3447)	(578.3445)	1025.6212(A')	1029.4518(A')	1026.1761(A')
615.0869(B_2)	616.3633(A'')	1032.1215(A'')	1032.1541(A'')	1039.4173(A'')
(615.0653)	(616.3736)	1094.9249(A')	1093.0491(A')	1109.8071(A')
660.7471(A_1)	657.6021(A')	1099.7331(A'')	1095.3915(A'')	1123.3530(A'')
(659.7126)	(657.6644)	1146.0798(A')	1129.1537(A')	1143.8162(A')
731.9785(B_1)	726.0628(A')	1155.9554(A'')	1139.7911(A'')	1154.0384(A'')
(730.7824)	(727.5602)	1196.0860(A')	1200.4612(A')	1192.5233(A')
732.3575(A_1)	730.0562(A')	1198.0969(A'')	1203.2940(A'')	1201.7957(A')
(734.4322)	(731.5808)	1205.3132(A')	1206.2435(A')	1209.6938(A'')
735.1062(B_2)	735.5187(A'')	1239.0489(A')	1224.6565(A'')	1226.7553(A')
(735.0732)	(735.4983)	1245.8649(A'')	1246.3801(A')	1239.0117(A'')
775.7371(A_2)	767.9193(A')	1260.7768(A'')	1265.8215(A'')	1244.5726(A')
(775.1297)	(769.8388)	1276.5522(A')	1266.8572(A')	1253.0595(A'')

786.0610(B ₁) (786.5876)	773.1437(A'') (773.6859)	1289.0121(A')	1320.1182(A')	1289.8817(A')
805.0391(A ₂) (805.0494)	799.5575(A'') (799.8639)	1296.6143(A'')	1325.4984(A'')	1304.2345(A'')
848.7606(B ₂) (848.5468)	851.8662(A'') (851.7593)	1348.1525(A')	1340.4184(A'')	1351.7674(A')
865.0581(B ₁) (865.3962)	855.2276(A')	1379.8061(A'')	1357.8555(A')	1352.3845(A'')
879.7938(A ₁) (878.8220)	877.7363(A')	1387.9277(A')	1378.7099(A'')	1377.3737(A'')
925.4745(A ₂) (925.3491)	891.2787(A')	1415.2328(A'')	1383.6330(A')	1398.8246(A')
933.7191(B ₁) (934.5118)	855.2276(A')	1472.9671(A'')	1460.8455(A'')	1479.8274(A'')
946.9202(B ₂) (946.9024)	(856.0465)	1501.9379(A')	1506.6883(A')	1493.4758(A')
1033.7918(A ₂) (1033.9488)	877.7363(A')	1529.9878(A'')	1524.8951(A'')	1523.0291(A'')
1035.3996(B ₁) (1035.4980)	(877.8155)	1560.7594(A')	1552.4840(A')	1569.5053(A')
1047.3004(A ₂) (1047.6948)	891.2787(A')	1572.5474(A'')	1558.3492(A'')	1570.0955(A'')
1057.1325(B ₁) (1055.9206)	(892.4628)	1664.1225(A')	1659.5546(A')	1675.5627(A'')
1065.4819(A ₂) (1064.0445)	916.2121(A'')	1676.5626(A'')	1671.2865(A'')	1678.7891(A')
1083.6602(A ₁) (1083.5043)	(916.2507)	1707.3765(A')	1700.4924(A')	1703.4984(A')
1094.1222(B ₂) (1093.9030)	937.8730(A')	1710.7751(A'')	1704.0873(A'')	1703.6599(A'')
1130.1302(B ₁) (1121.9979)	(938.6684)	1732.9330(A')	1720.0501(A')	1768.5532(A')
1165.5929(A ₁) (1165.4575)	945.2957(A'')	3167.8306(A')	3135.0321(A')	3105.2145(A')
1166.4713(B ₂) (1166.3428)	(945.2636)	3213.6482(A'')	3214.7431(A'')	3198.6671(A'')
1202.5210(A ₁) (1202.5368)	1023.5242(A'')	3215.8169(A')	3226.8037(A')	3214.2746(A')
1211.3501(B ₂) (1211.3458)	(1023.8249)	3215.9592(A'')	3227.4439(A'')	3218.3462(A'')
1225.4192(A ₁) (1225.0376)	1030.3894(A')	3227.9299(A')	3233.9526(A')	3221.4642(A')
1243.2260(A ₁) (1243.0304)	(1030.2367)	3228.1984(A'')	3244.5471(A'')	3225.6179(A'')
1257.8771(B ₂) (1257.3377)	1042.7651(A'')	3232.6806(A')	3244.6810(A')	3226.9764(A')
1293.9515(B ₂) (1293.3797)	(1042.9583)	3228.1984(A'')	3251.7747(A'')	3243.5218(A'')
1316.1677(A ₁) (1315.6748)	1045.8306(A')	3232.6806(A')	3252.0601(A')	3243.6483(A')
1360.4504(A ₁) (1360.1273)	(1046.3258)	3238.3709(A'')	3266.0659(A'')	3282.2868(A'')
1394.3049(B ₂)	1053.7174(A'')	3239.1360(A')	3266.2298(A')	3283.4280(A')
	(1052.1168)	3243.9503(A'')		
	1084.1662(A')	3244.3869(A')		
	(1084.1587)			
	1095.2788(A'')			
	(1095.2739)			
	1167.8796(A'')			
	(1168.0397)			
	1168.8787(A')			
	(1169.0377)			
	1203.5220(A')			
	(1203.6119)			
	1210.3880(A'')			
	(1210.4925)			
	1226.2219(A')			
	(1226.1954)			
	1240.5812(A')			
	(1240.6531)			
	1254.1647(A'')			
	(1253.9288)			
	1291.0839(A'')			
	(1290.9523)			
	1309.7318(A')			
	(1309.7498)			
	1360.7113(A')			
	(1360.7366)			
	1382.6177(A'')			

(1393.9618)	(1382.3750)			
1432.3924(A ₁)	1430.7984(A')			
(1432.4430)	(1430.9107)			
1463.0947(B ₂)	1454.2448(A'')			
(1462.8771)	(1454.2741)			
1475.3817(B ₂)	1471.2511(A'')			
(1474.9214)	(1471.0861)			
1487.4517(A ₁)	1487.6148(A')			
(1487.3254)	(1487.6980)			
1540.7781(B ₂)	1536.4046(A'')			
(1540.2180)	(1536.0931)			
1545.9709(A ₁)	1543.8093(A')			
(1545.6586)	(1543.8440)			
1574.3332(B ₂)	1569.7487(A'')			
(1574.0036)	(1569.7730)			
1598.6810(A ₁)	1605.7328(A')			
(1598.6244)	(1605.6791)			
1630.6988(B ₂)	1613.7912(A'')			
(1630.6755)	(1613.4355)			
1663.1086(B ₂)	1645.6170(A'')			
(1661.8309)	(1645.2657)			
1696.3596(A ₁)	1697.2177(A')			
(1696.4268)	(1697.2898)			
1697.0237(B ₂)	1697.7172(A'')			
(1696.9854)	(1697.7609)			
1702.8378(A ₁)	1708.1695(A')			
(1702.9693)	(1708.0805)			
2950.2955(A ₁) ^c	3191.2546(A')			
(2937.6396)	(3195.1413)			
3183.0869(B ₂)	3207.2994(A'')			
(3183.2016)	(3206.2613)			
3200.3110(A ₁)	3207.9577(A'')			
(3200.3983)	(3209.0780)			
3202.8350(B ₂)	3211.5213(A')			
(3202.8351)	(3213.0685)			
3207.1732(A ₁)	3222.8150(A')			
(3207.1257)	(3222.4268)			
3230.9658(B ₂)	3223.5783(A'')			
(3231.1025)	(3223.6324)			
3231.1907(A ₁)	3225.4061(A')			
(3231.3239)	(3224.7716)			
3243.6208(B ₂)	3250.6967(A'')			
(3243.7453)	(3251.0232)			
3243.6900(A ₁)	3250.8420(A')			
(3243.8135)	(3251.1537)			
3258.4071(B ₂)	3268.6329(A'')			
(3258.4483)	(3269.2447)			
3258.4256(A ₁)	3268.6767(A')			
(3258.4674)	(3269.2871)			

^aIntermolecular modes; ^bValues in parenthesis have been obtained with BSSE; ^cVery intense C–H stretching mode characteristic of the C⁺–H•••Cl[−] hydrogen bond.

Table S8. Vibrational frequencies (in cm⁻¹) computed at the M05-2X/6-311++G** level.

radical	cation	HBCIP	TS1	cov1	cov2	TS2
46.5764(B ₁)	64.7789(B ₁)	44.0003(B ₁) ^a	-57.0353(A')	52.9440(A')	57.0037(A')	-68.5425(A')
92.5932(A ₂)	84.5433(A ₂)	(39.8923) ^b	(-63.8121)	94.6839(A'')	92.8623(A'')	61.4736(A'')
194.0179(B ₁)	194.8002(B ₁)	64.3940(B ₂) ^a	54.4029(A')	113.6001(A')	129.1082(A')	85.4027(A')
202.3275(A ₂)	195.6607(A ₂)	(58.7195)	(54.4329)	125.7479(A'')	177.3693(A'')	192.5957(A'')
243.5622(A ₁)	244.5633(A ₁)	70.3045(B ₁) ^a	70.9084(A'')	181.4661(A')	190.6275(A')	205.7474(A')
294.7371(B ₁)	337.9234(B ₂)	(65.0808)	(69.4031)	243.8239(A'')	230.7254(A'')	253.7655(A')
336.6118(B ₂)	338.0599(B ₁)	94.3054(A ₂)	97.6245(A'')	274.9119(A')	263.9995(A')	292.1232(A'')
338.4550(A ₁)	348.0097(A ₁)	(92.9121)	(95.5137)	324.3909(A')	318.7422(A')	293.8850(A')
393.6399(A ₂)	380.3132(A ₂)	164.8284(A ₁) ^a	145.3812(A')	325.9150(A'')	320.3865(A'')	331.3052(A'')
439.8138(B ₁)	435.2217(B ₁)	(157.9132)	(145.6710)	344.6925(A')	394.1601(A'')	366.1910(A')
502.1681(A ₂)	481.4252(A ₂)	194.1977(A ₂)	192.5517(A'')	397.0913(A'')	413.2174(A')	392.9448(A'')
509.5256(B ₂)	506.8443(B ₂)	(193.9575)	(193.7658)	465.3809(A')	462.7556(A')	437.2359(A')
527.2416(A ₁)	526.5104(A ₁)	196.2900(B ₁)	208.0301(A')	481.4258(A'')	469.0123(A'')	485.6322(A')
548.4257(B ₁)	542.3005(B ₁)	(196.2853)	(208.0296)	532.0550(A'')	490.5055(A')	489.3044(A'')
590.3550(A ₂)	567.3230(A ₂)	255.4307(A ₁) ^a	239.4909(A')	532.1642(A')	519.3090(A'')	528.2301(A'')
625.4441(B ₂)	619.3113(B ₂)	(252.5487)	(239.0849)	545.0445(A')	555.9507(A')	550.0363(A')
663.5346(A ₁)	661.1286(A ₁)	333.6841(B ₁)	336.8755(A'')	596.1332(A'')	597.7904(A'')	594.1330(A'')
718.2378(B ₁)	723.7617(A ₁)	(332.7451)	(336.8014)	630.4258(A'')	613.0000(A'')	632.3117(A'')
723.4230(A ₁)	728.7921(B ₁)	340.3431(B ₂)	339.0207(A')	653.6915(A')	642.3308(A')	645.1045(A')
737.6981(B ₂)	736.1269(B ₂)	(339.9358)	(338.0000)	723.6036(A'')	715.4880(A'')	683.7347(A')
747.5997(B ₁)	760.0507(A ₂)	351.4041(A ₁) ^a	370.1051(A')	724.2751(A')	727.6540(A')	738.5708(A'')
765.1377(A ₂)	777.3353(B ₁)	(350.4045)	(366.8764)	737.4603(A')	755.0972(A')	738.9318(A')
776.1074(A ₂)	797.2854(A ₂)	385.3142(A ₂)	386.5005(A'')	750.4092(A')	763.6229(A'')	746.1263(A')
817.0989(B ₁)	840.4998(B ₂)	(385.0392)	(387.0605)	772.6003(A'')	793.6623(A'')	765.3306(A'')
836.2563(B ₁)	860.3011(B ₁)	442.4709(B ₁)	443.7715(A')	789.4062(A'')	794.9854(A')	790.5577(A'')
843.4014(B ₂)	884.0325(A ₁)	(440.6913)	(441.4834)	816.2099(A')	819.0028(A')	809.0739(A')
874.4829(A ₁)	903.4668(A ₂)	487.6857(A ₂)	483.0307(A'')	829.9837(A')	833.0560(A')	830.1100(A')
887.2909(A ₂)	923.4449(B ₁)	(487.0156)	(485.7943)	852.2957(A'')	854.9831(A'')	849.2827(A'')
901.7196(B ₁)	948.2341(B ₂)	507.0924(B ₂)	507.9428(A'')	874.0550(A')	891.8180(A')	855.5444(A')
944.1655(B ₂)	994.1002(B ₁)	(506.9814)	(507.8053)	907.4124(A'')	899.2202(A'')	899.2937(A'')
975.8359(A ₂)	1016.9825(A ₂)	526.5616(A ₁)	521.6482(A')	918.0454(A')	914.4992(A'')	915.8892(A')
980.7720(B ₁)	1029.8255(B ₁)	(526.1443)	(521.4768)	930.0842(A'')	922.9742(A')	923.2949(A'')
1005.7976(A ₂)	1044.0129(A ₂)	545.2418(B ₁)	545.1179(A')	986.5768(A'')	991.6417(A'')	992.8332(A'')
1006.2238(B ₁)	1046.4671(B ₁)	(544.7943)	(544.0979)	988.8803(A')	995.3450(A')	996.1366(A')
1030.4209(A ₂)	1053.1799(A ₂)	578.0484(A ₂)	576.2308(A'')	1019.4586(A'')	1020.9136(A'')	1018.7393(A'')
1086.7081(A ₁)	1076.0015(A ₁)	(577.8162)	(577.5186)	1021.3292(A')	1022.8410(A')	1020.2928(A')
1095.1129(B ₂)	1085.7645(B ₂)	617.8285(B ₂)	618.9468(A'')	1026.0933(A'')	1027.6128(A'')	1031.7933(A'')
1154.9403(B ₂)	1171.0946(B ₂)	(617.8060)	(618.9572)	1090.8722(A')	1089.1034(A')	1105.7847(A')
1158.9511(A ₁)	1173.9535(A ₁)	662.2845(A ₁)	659.2956(A')	1095.5478(A'')	1091.3454(A'')	1119.4751(A'')
1176.5145(B ₂)	1209.8567(A ₁)	(661.1925)	(659.2653)	1145.7274(A')	1129.7995(A')	1144.3093(A')
1190.6919(A ₁)	1212.6278(B ₂)	732.0678(A ₁)	725.5055(A')	1154.2265(A'')	1137.6595(A'')	1152.5252(A'')
1202.2877(A ₁)	1221.8955(A ₁)	(730.4911)	(726.6190)	1193.6150(A')	1198.0665(A')	1190.4914(A')
1210.9591(B ₂)	1233.7051(B ₂)	733.5743(B ₁)	729.2318(A')	1195.9869(A'')	1200.8893(A'')	1201.0668(A')
1226.5444(A ₁)	1242.2292(A ₁)	(732.9741)	(729.6026)	1203.3966(A')	1203.7226(A')	1209.3169(A'')
1272.5514(B ₂)	1282.1041(B ₂)	735.2786(B ₂)	735.7610(A'')	1234.7626(A')	1222.3912(A'')	1222.1369(A')
1279.2171(A ₁)	1304.6710(A ₁)	(735.3882)	(735.7875)	1241.8477(A'')	1243.6741(A')	1235.9671(A'')
1327.0398(B ₂)	1369.3679(A ₁)	769.3002(A ₂)	768.2844(A'')	1259.8435(A'')	1261.1018(A')	1241.6102(A')
1342.0180(A ₁)	1378.9245(B ₂)	(768.6655)	(768.5312)	1272.5839(A')	1261.2863(A'')	1249.8099(A'')
1382.7287(A ₁)	1442.7320(A ₁)	783.4784(B ₁)	769.4617(A')	1285.6868(A')	1317.8956(A')	1287.1089(A')

1386.7698(B ₂)	1457.2725(B ₂)	(783.8584)	(769.0808)	1292.0590(A'')	1319.2249(A'')	1303.1055(A'')
1452.8942(B ₂)	1465.9395(B ₂)	803.7095(A ₂)	800.6143(A'')	1345.5231(A')	1337.2915(A'')	1345.4305(A')
1458.1050(B ₂)	1481.3838(A ₁)	(803.3843)	(801.6190)	1365.0304(A'')	1355.6028(A')	1352.4646(A'')
1477.3862(A ₁)	1525.5227(B ₂)	847.7336(B ₂)	850.5978(A'')	1373.6439(A')	1365.5493(A'')	1364.1751(A'')
1507.7676(B ₂)	1536.9776(A ₁)	(847.4906)	(850.4178)	1413.6281(A'')	1375.4919(A')	1391.1316(A')
1532.0020(A ₁)	1555.0989(B ₂)	864.1764(B ₁)	853.4160(A')	1467.0632(A'')	1454.6980(A'')	1476.9781(A'')
1555.1108(B ₂)	1582.2052(A ₁)	(863.8917)	(851.6452)	1495.8968(A')	1500.7275(A')	1488.8931(A')
1621.4768(A ₁)	1595.1222(B ₂)	883.0846(A ₁)	881.1234(A')	1522.8779(A'')	1517.7855(A'')	1517.1615(A'')
1631.8632(B ₂)	1639.0417(B ₂)	(882.1022)	(880.8649)	1552.6351(A')	1544.3130(A')	1562.9984(A'')
1669.7735(B ₂)	1681.7735(A ₁)	919.0555(A ₂)	894.2840(A')	1564.1045(A'')	1549.4934(A'')	1563.1884(A')
1673.1437(A ₁)	1689.7305(B ₂)	(918.6661)	(888.9530)	1654.8183(A')	1649.5158(A')	1666.1697(A'')
1715.4750(A ₁)	1694.5182(A ₁)	928.5785(B ₁)	911.2321(A'')	1667.3492(A'')	1661.6697(A'')	1670.0001(A')
3167.7032(B ₂)	3187.6375(B ₂)	(928.4464)	(911.3866)	1697.0038(A')	1689.5885(A')	1693.7938(A')
3188.1600(A ₁)	3187.9363(A ₁)	950.7809(B ₂)	932.2121(A')	1700.2477(A'')	1693.1024(A'')	1694.0064(A'')
3198.2488(A ₁)	3202.5662(A ₁)	(950.7888)	(931.4520)	1722.0465(A')	1708.0370(A')	1758.9847(A')
3207.9926(B ₂)	3224.9357(B ₂)	1029.9380(A ₂)	949.1788(A'')	3162.7358(A')	3128.2982(A')	3102.2981(A')
3209.8797(A ₁)	3225.4999(A ₁)	(1029.8530)	(949.1862)	3196.2497(A'')	3196.5126(A'')	3188.3718(A'')
3215.7503(B ₂)	3233.8764(B ₂)	1031.2057(B ₁)	1024.0778(A'')	3209.6040(A')	3212.9226(A')	3206.7324(A')
3216.2816(A ₁)	3234.3087(A ₁)	(1031.4909)	(1024.3085)	3209.8545(A'')	3214.3136(A'')	3214.9442(A'')
3225.0150(B ₂)	3239.3525(B ₂)	1042.4527(A ₂)	1030.7002(A')	3214.1467(A')	3216.5616(A')	3216.7430(A')
3226.3473(A ₁)	3239.7199(A ₁)	(1042.7910)	(1031.1873)	3215.2051(A'')	3231.3193(A'')	3224.5380(A'')
3242.0011(B ₂)	3248.8051(A ₁)	1059.0930(B ₁)	1042.9341(A'')	3217.2622(A')	3231.3984(A')	3224.8137(A')
3242.0110(A ₁)	3248.8092(B ₂)	(1058.4070)	(1044.0276)	3225.9483(A'')	3243.7774(A'')	3240.6091(A'')
		1067.1953(A ₂)	1046.7661(A')	3226.1967(A')	3243.9470(A')	3240.7177(A')
		(1065.6837)	(1047.8220)	3238.4534(A'')	3254.2897(A'')	3277.3698(A'')
		1079.2821(A ₁)	1047.8884(A'')	3238.5838(A')	3254.5945(A')	3278.5340(A')
		(1079.0712)	(1048.0582)			
		1090.1149(B ₂)	1080.2331(A')			
		(1089.7949)	(1080.0176)			
		1144.0118(B ₁)	1091.7298(A'')			
		(1135.5862)	(1091.5608)			
		1163.2119(A ₁)	1165.1639(A'')			
		(1163.2197)	(1165.2989)			
		1163.6995(B ₂)	1166.8294(A')			
		(1163.7350)	(1166.9199)			
		1198.4130(A ₁)	1201.0670(A')			
		(1198.3112)	(1201.1086)			
		1208.4437(B ₂)	1209.3142(A'')			
		(1208.3372)	(1209.3929)			
		1218.9637(A ₁)	1220.3935(A')			
		(1218.8581)	(1220.3807)			
		1239.7709(A ₁)	1237.6967(A')			
		(1239.4167)	(1237.6968)			
		1251.6439(B ₂)	1249.2332(A'')			
		(1251.2074)	(1248.7042)			
		1289.6665(B ₂)	1288.4768(A'')			
		(1289.1620)	(1288.1357)			
		1311.8802(A ₁)	1306.8596(A')			
		(1311.0160)	(1306.7379)			
		1357.0183(A ₁)	1357.1070(A')			
		(1356.7924)	(1357.1044)			
		1387.0730(B ₂)	1377.7395(A'')			
		(1386.8590)	(1377.2641)			

	1421.1946(A ₁) (1421.1241)	1419.4987(A') (1419.4765)		
	1456.6842(B ₂) (1456.3668)	1446.3045(A'') (1445.8693)		
	1468.5703(B ₂) (1468.2344)	1467.1273(A'') (1466.7728)		
	1480.8354(A ₁) (1480.6501)	1481.7994(A') (1481.8902)		
	1535.2792(B ₂) (1534.9192)	1532.8477(A'') (1532.3192)		
	1537.5798(A ₁) (1537.1262)	1535.6469(A') (1535.6327)		
	1565.8602(B ₂) (1565.5309)	1561.5258(A'') (1561.5956)		
	1588.8751(A ₁) (1588.7973)	1595.9817(A') (1595.8851)		
	1621.7788(B ₂) (1621.7310)	1608.1259(A'') (1607.3654)		
	1656.2446(B ₂) (1655.3450)	1638.8475(A'') (1637.8759)		
	1687.0936(A ₁) (1687.1723)	1686.9174(A') (1686.9522)		
	1687.2923(B ₂) (1687.3683)	1687.1192(A'') (1687.1060)		
	1692.2033(A ₁) (1692.1627)	1696.7406(A') (1696.6855)		
	2916.8874(A ₁) ^c (2902.2230)	3164.3665(A') (3167.3446)		
	3177.1511(B ₂) (3177.5326)	3190.6794(A'') (3191.5317)		
	3177.6829(B ₂) (3179.3452)	3193.8520(A') (3194.7548)		
	3182.0914(A ₁) (3183.9930)	3196.9902(A'') (3196.0419)		
	3195.0260(A ₁) (3195.0528)	3213.6258(A') (3212.8345)		
	3219.7848(B ₂) (3219.7185)	3218.7429(A'') (3218.8245)		
	3219.9838(A ₁) (3219.9223)	3219.6125(A') (3219.5457)		
	3229.8236(B ₂) (3229.6781)	3234.3603(A'') (3234.4881)		
	3229.8376(A ₁) (3229.6933)	3234.5070(A') (3234.6190)		
	3239.8327(B ₂) (3239.7517)	3253.3006(A'') (3254.2068)		
	3239.8754(A ₁) (3239.7970)	3253.3474(A') (3254.2513)		

^aIntermolecular modes; ^bValues in parenthesis have been obtained with BSSE; ^cVery intense C–H stretching mode characteristic of the C⁺–H•••Cl[−] hydrogen bond.

Table S9. Vibrational frequencies (in cm^{-1}) computed at the MP2/6-31++G** level.

HBCIP(C_s)	TS1(C_s)	cov1(C_s)	cov2(C_s)	TS2(C_s)
42.9510(A') ^a	-94.4680(A')	53.4780(A')	56.6255(A')	-62.0760(A')
(42.9965) ^b	(-76.2653)	96.1865(A'')	94.0046(A'')	59.6832(A'')
51.2812(A'') ^a	44.2879(A')	113.9206(A')	126.5697(A')	88.4025(A')
(54.9920)	(51.7512)	126.1571(A'')	169.8171(A'')	182.4520(A'')
66.6100(A') ^a	50.6379(A'')	176.5219(A')	184.0977(A')	193.3589(A')
(60.4461)	(58.3275)	238.0413(A'')	223.4304(A'')	253.0869(A')
81.3567(A'')	81.6540(A'')	271.4575(A')	259.9503(A')	288.4141(A'')
(81.8945)	(82.9564)	314.9573(A')	305.9695(A')	294.9187(A')
162.8029(A') ^a	121.8761(A')	318.8624(A'')	314.2395(A'')	330.2192(A'')
(151.6398)	(123.3382)	343.9088(A')	367.8170(A'')	354.5675(A')
168.9898(A'')	162.6974(A'')	373.5523(A'')	412.4992(A')	362.6566(A'')
(174.7172)	(169.3478)	443.4589(A')	431.6585(A'')	422.5394(A')
171.9147(A')	170.9986(A')	457.2459(A'')	438.3546(A')	443.4339(A')
(178.3759)	(177.9581)	485.6713(A')	452.8860(A')	448.2559(A'')
249.3512(A') ^a	233.3141(A')	500.1660(A'')	456.2709(A'')	501.0248(A'')
(247.4446)	(234.8704)	524.5535(A'')	483.4969(A')	517.1518(A')
284.7534(A')	245.6727(A')	532.2348(A')	505.0069(A'')	522.1981(A'')
(297.2177)	(318.7312)	585.0264(A')	554.9407(A')	549.1993(A')
332.4182(A'')	297.7233(A'')	593.7309(A'')	572.7399(A'')	574.3199(A'')
(337.6881)	(330.1544)	629.2830(A'')	607.1085(A'')	626.6604(A'')
338.8882(A'')	315.5738(A')	662.9972(A')	647.4342(A')	657.1215(A')
(343.8630)	(342.4568)	720.4008(A'')	716.6461(A'')	710.7537(A')
350.7686(A') ^a	331.3737(A'')	732.4978(A')	733.2106(A')	739.0549(A'')
(349.7181)	(351.6877)	732.6782(A')	745.7622(A'')	742.1834(A'')
393.8571(A')	337.7365(A'')	750.5111(A'')	775.1251(A')	750.3866(A')
(397.7079)	(390.2494)	787.1218(A')	792.0736(A')	763.2954(A')
416.0952(A'')	351.5135(A')	805.3623(A')	801.4133(A')	793.5481(A')
(425.9387)	(402.6747)	829.1749(A'')	828.6458(A'')	829.1334(A'')
442.0348(A')	388.9972(A'')	835.8541(A')	834.4249(A')	830.8614(A')
(463.6063)	(432.3939)	837.5264(A'')	838.6763(A'')	838.1202(A'')
456.7202(A'')	396.9024(A')	875.4456(A')	885.2865(A'')	859.4210(A')
(477.8297)	(438.4361)	891.9327(A'')	889.1455(A')	889.5222(A'')
502.7680(A'')	440.3066(A')	897.4004(A')	890.5403(A'')	897.3636(A')
(503.5880)	(471.8214)	901.3185(A'')	893.4284(A')	906.2846(A'')
526.7012(A')	443.5415(A'')	904.4930(A')	899.3532(A')	909.4649(A')
(526.5333)	(503.0778)	925.7393(A'')	903.9977(A'')	916.2962(A'')
530.3746(A'')	503.3156(A'')	961.7371(A'')	968.9427(A'')	929.3695(A'')
(610.9785)	(503.7602)	1074.7474(A')	1073.5975(A')	1089.1799(A')
615.6044(A'')	518.8863(A')	1080.8437(A'')	1076.6555(A'')	1106.3724(A'')
(636.3664)	(521.6544)	1140.6806(A')	1123.4415(A')	1142.3724(A')
659.9772(A')	616.2614(A'')	1149.3104(A'')	1133.4174(A'')	1147.6711(A'')
(659.1239)	(616.7571)	1199.6473(A')	1195.8564(A')	1185.5713(A')
677.9571(A')	654.3664(A')	1204.4350(A')	1202.6119(A')	1199.3066(A')
(705.6545)	(655.6164)	1205.2653(A'')	1204.4839(A'')	1211.9675(A'')
726.5514(A')	675.3704(A')	1233.6274(A')	1222.4377(A'')	1231.0726(A')
(733.0390)	(679.8102)	1250.5586(A'')	1234.9749(A')	1239.0545(A'')
736.3676(A'')	719.0440(A')	1261.7772(A'')	1262.7629(A'')	1259.9786(A')
(736.7546)	(717.7920)	1277.3780(A')	1271.3556(A')	1262.0754(A'')
744.4186(A')	735.8735(A')	1284.0955(A'')	1302.5453(A'')	1291.0267(A')

(756.3684)	(734.7213)	1301.7408(A')	1303.7884(A')	1296.8657(A'')
756.7257(A'')	736.4860(A'')	1345.5387(A')	1331.3513(A'')	1343.9527(A'')
(761.5327)	(736.3846)	1394.9415(A'')	1335.7071(A')	1361.5741(A')
806.9885(A')	738.8156(A'')	1462.8126(A'')	1454.5875(A'')	1466.3292(A'')
(819.0969)	(737.1276)	1475.9868(A')	1474.7376(A')	1471.0225(A'')
840.0789(A'')	788.3663(A')	1488.3615(A')	1479.1559(A'')	1472.4222(A')
(839.3916)	(796.3851)	1489.3696(A'')	1492.6929(A')	1478.6688(A')
859.7339(A')	824.5509(A'')	1511.2335(A'')	1508.7168(A'')	1513.4718(A'')
(864.6636)	(820.6967)	1533.8390(A')	1525.0291(A')	1543.7316(A')
859.7361(A'')	828.3928(A')	1548.4567(A'')	1535.2344(A'')	1546.0700(A'')
(869.4296)	(828.9209)	1619.7920(A')	1614.5561(A')	1632.8208(A'')
881.9562(A')	838.6034(A'')	1632.6496(A'')	1627.7605(A'')	1635.5557(A')
(881.2508)	(839.3017)	1657.0422(A')	1654.5902(A')	1656.3066(A')
902.5313(A'')	878.7697(A')	1662.5712(A'')	1662.8198(A'')	1658.0741(A'')
(909.5007)	(879.4664)	1681.2926(A')	1671.2788(A')	1720.6575(A')
908.4708(A')	889.4793(A'')	3164.3804(A')	3126.8150(A')	3109.5138(A')
(920.9712)	(896.2282)	3208.9847(A'')	3209.1480(A'')	3207.6736(A'')
919.4702(A'')	896.6343(A')	3229.3848(A')	3229.4509(A')	3229.6605(A')
(929.8353)	(900.0669)	3235.2831(A'')	3238.1052(A'')	3241.2567(A'')
948.4806(A'')	904.9068(A'')	3235.8758(A')	3238.3851(A')	3242.1693(A')
(948.2443)	(912.2830)	3239.5480(A'')	3252.6913(A'')	3255.5059(A'')
964.2232(A'')	928.4352(A'')	3239.9367(A')	3252.7554(A')	3255.5715(A')
(970.0048)	(915.1336)	3257.1823(A'')	3267.9789(A'')	3272.0027(A'')
970.9971(A')	931.6098(A')	3257.2769(A')	3268.1586(A')	3272.1681(A')
(971.2641)	(918.4705)	3271.7795(A'')	3279.4583(A'')	3308.6480(A'')
1066.7227(A')	943.9094(A'')	3271.9545(A')	3279.8413(A')	3309.8787(A')
(1055.1860)	(945.0666)			
1076.9779(A'')	1069.2241(A')			
(1067.4196)	(1069.4517)			
1100.0027(A')	1080.3477(A'')			
(1077.9290)	(1080.8681)			
1162.2491(A'')	1163.1645(A'')			
(1162.6125)	(1164.0949)			
1163.2391(A')	1165.7015(A'')			
(1163.9172)	(1166.9150)			
1207.5143(A')	1207.7809(A')			
(1207.5199)	(1208.0587)			
1217.6384(A'')	1216.5336(A'')			
(1217.8550)	(1216.9881)			
1223.6936(A')	1223.3444(A')			
(1224.5030)	(1224.2247)			
1255.6671(A')	1248.0885(A')			
(1255.4620)	(1248.0848)			
1282.7006(A'')	1272.0647(A'')			
(1282.6995)	(1272.7984)			
1289.5445(A'')	1285.3542(A'')			
(1290.1011)	(1286.1667)			
1318.6583(A')	1307.1790(A')			
(1318.8104)	(1308.0470)			
1368.1679(A')	1366.8269(A')			
(1368.1182)	(1367.6538)			
1415.2597(A'')	1392.3400(A'')			
(1412.7160)	(1391.6273)			

1458.7494(A'')	1454.7402(A'')			
(1458.4103)	(1455.3527)			
1472.7514(A')	1470.0488(A')			
(1472.6368)	(1470.7470)			
1518.7766(A')	1515.8806(A')			
(1519.2790)	(1516.8085)			
1522.1871(A'')	1519.2031(A'')			
(1522.6422)	(1519.6941)			
1526.3989(A')	1522.2126(A')			
(1526.2492)	(1523.1278)			
1556.7742(A'')	1535.3205(A'')			
(1553.9484)	(1533.9355)			
1560.6306(A')	1568.5136(A')			
(1561.7260)	(1569.5276)			
1576.0849(A'')	1568.5166(A'')			
(1574.5121)	(1569.6001)			
1633.7908(A'')	1619.6874(A'')			
(1630.4202)	(1619.5807)			
1647.0032(A')	1644.1188(A'')			
(1647.7906)	(1645.5361)			
1656.2072(A'')	1652.4737(A')			
(1654.6576)	(1653.0337)			
1671.2954(A')	1671.3138(A')			
(1671.0529)	(1671.8930)			
1708.6752(A'')	1688.0468(A'')			
(1704.5417)	(1688.9558)			
2911.0269(A') ^c	3208.3158(A'')			
(2941.0820)	(3209.0929)			
3200.4783(A'')	3226.9652(A')			
(3203.2471)	(3228.4925)			
3205.0149(A')	3228.0891(A')			
(3207.2306)	(3244.6130)			
3206.8647(A'')	3245.5162(A'')			
(3207.8530)	(3246.9934)			
3226.2024(A')	3245.9934(A')			
(3226.9309)	(3247.4678)			
3246.2785(A'')	3250.0527(A'')			
(3246.5959)	(3257.5024)			
3246.4559(A')	3251.7067(A')			
(3246.7849)	(3259.0239)			
3263.0329(A'')	3264.0339(A'')			
(3263.4710)	(3265.6055)			
3263.0861(A')	3264.1708(A')			
(3263.5194)	(3265.9769)			
3277.8593(A'')	3278.2481(A'')			
(3278.3366)	(3279.6813)			
3277.9356(A')	3278.3538(A')			
(3278.4087)	(3279.8144)			

^aIntermolecular modes; ^bValues in parenthesis have been obtained with BSSE; ^cVery intense C–H stretching mode characteristic of the C⁺–H•••Cl[−] hydrogen bond.

Table S10. Vibrational frequencies (in cm^{-1}) computed at the MP2/6-311++G**(H,Cl)/6-31++G**(C) level.

HBCIP(C_s)	TS1(C_s)	cov1(C_s)	cov2(C_s)	TS2(C_s)
42.7435(A') ^a	-98.5053(A')	53.0987(A')	56.6985(A')	-64.1774(A')
(42.3698) ^b	(-76.4272)	96.4400(A'')	93.5157(A'')	57.5573(A'')
58.6138(A'') ^a	48.2027(A')	113.5794(A')	125.6096(A')	86.9979(A')
(55.9333)	(52.8937)	125.5792(A'')	169.1352(A'')	181.1233(A'')
66.3255(A') ^a	53.8870(A'')	176.5271(A')	184.7515(A')	192.2229(A')
(61.7238)	(59.7814)	237.0435(A'')	223.1160(A'')	251.3718(A')
81.8959(A'')	87.2528(A'')	270.4362(A')	259.4338(A')	285.2993(A'')
(82.1921)	(83.7689)	312.2597(A')	304.2155(A')	293.7158(A')
161.8965(A') ^a	122.4690(A')	317.4955(A'')	314.0533(A'')	328.4218(A'')
(150.3402)	(126.7308)	342.9345(A')	363.8051(A'')	350.8910(A')
170.9948(A'')	164.9597(A'')	370.1930(A'')	402.1277(A'')	355.9101(A'')
(175.5825)	(171.6848)	436.3180(A'')	408.7156(A')	416.4899(A')
173.2260(A')	173.2813(A')	437.7469(A')	411.7792(A')	424.1557(A'')
(180.0513)	(180.5029)	446.7718(A')	426.5617(A'')	429.5229(A')
246.9433(A') ^a	232.6412(A')	476.8015(A'')	434.4925(A')	470.2448(A')
(245.4928)	(234.1787)	519.0605(A'')	473.5741(A')	475.9476(A'')
281.9145(A')	277.5593(A')	530.6120(A')	503.4520(A'')	517.5258(A'')
(297.2741)	(312.3549)	575.7020(A')	550.7491(A')	536.9727(A'')
328.4564(A'')	313.9336(A'')	589.9523(A'')	571.2877(A'')	547.2589(A')
(336.0088)	(329.9643)	626.1249(A'')	604.2395(A'')	623.4272(A'')
337.1540(A'')	318.4410(A')	661.2369(A')	642.8617(A')	653.4105(A')
(338.6599)	(337.0815)	716.3313(A'')	712.0738(A'')	702.0947(A')
349.7613(A') ^a	332.8132(A'')	725.1171(A')	725.4269(A')	730.4244(A'')
(348.7268)	(349.8660)	731.2520(A')	737.9529(A'')	736.3800(A'')
391.9142(A')	335.3350(A'')	742.8501(A'')	772.6358(A')	742.2165(A')
(397.6620)	(385.3614)	779.7316(A')	785.6832(A')	755.8005(A')
412.6406(A'')	349.7873(A')	802.9204(A')	797.6309(A')	786.3965(A')
(423.4751)	(405.6049)	821.5230(A'')	819.4698(A'')	816.7350(A'')
435.4225(A')	388.5121(A')	826.3171(A')	823.8597(A')	818.5355(A')
(459.1768)	(427.9503)	833.9051(A'')	836.9808(A'')	835.6845(A'')
448.1300(A'')	389.2185(A'')	870.9287(A')	874.4156(A'')	853.9008(A')
(471.2348)	(439.5905)	879.7791(A'')	878.0062(A')	878.5184(A')
500.9454(A'')	408.4980(A')	885.1680(A')	881.6062(A'')	887.3108(A')
(501.3392)	(497.8840)	890.4739(A'')	883.9226(A')	889.9599(A'')
524.7586(A')	427.9105(A'')	895.0543(A')	893.9648(A')	893.2320(A')
(524.7934)	(501.7064)	920.4392(A'')	898.0965(A'')	908.3175(A'')
552.4119(A'')	500.9306(A'')	952.4442(A'')	963.5769(A'')	921.1333(A'')
(610.2793)	(520.8324)	1071.3936(A')	1070.3306(A')	1086.3928(A')
614.6542(A'')	517.6863(A')	1076.5501(A'')	1073.0490(A'')	1100.8084(A'')
(656.2001)	(552.5940)	1133.9599(A')	1118.1553(A')	1136.5377(A')
656.1177(A')	613.4503(A'')	1141.8523(A'')	1127.5918(A'')	1141.5503(A'')
(657.8715)	(614.6002)	1189.7731(A')	1188.5953(A')	1180.2502(A')
675.9122(A')	627.3275(A')	1190.6890(A'')	1189.0799(A')	1189.4977(A')
(706.1556)	(653.8187)	1193.2394(A')	1190.4031(A'')	1197.1301(A'')
725.3791(A')	654.0139(A')	1230.5971(A')	1214.7800(A'')	1219.7522(A')
(730.3577)	(669.2969)	1245.8501(A'')	1231.3965(A')	1232.0470(A'')
733.9861(A'')	715.9138(A')	1256.5895(A'')	1256.2218(A'')	1254.2710(A'')
(734.2406)	(717.1052)	1267.7565(A')	1262.4085(A')	1256.0762(A')

738.5467(A')	722.5532(A')	1277.5649(A'')	1299.2649(A'')	1277.7768(A')
(754.6622)	(727.7861)	1297.8060(A')	1299.5741(A')	1283.0177(A'')
748.8006(A'')	727.3887(A'')	1340.3258(A')	1322.7172(A'')	1329.1646(A'')
(759.2719)	(728.0547)	1386.3328(A'')	1335.9966(A')	1344.8806(A')
799.0911(A')	734.0895(A'')	1451.9888(A'')	1443.0066(A'')	1452.1902(A'')
(812.6327)	(734.6878)	1468.3915(A')	1469.3974(A')	1462.5088(A')
837.7938(A'')	782.3954(A')	1486.5903(A')	1477.8567(A'')	1470.2144(A'')
(837.3232)	(789.6712)	1487.2899(A'')	1488.5730(A')	1476.3960(A')
854.0687(A'')	813.6022(A'')	1505.1708(A'')	1501.4923(A'')	1500.5660(A'')
(860.3671)	(815.2748)	1525.6159(A')	1518.0993(A')	1533.5128(A')
854.7139(A')	818.7739(A')	1541.2626(A'')	1529.5318(A'')	1538.0953(A'')
(866.8369)	(826.2429)	1616.9018(A')	1611.6490(A')	1629.2604(A'')
876.6748(A')	836.6710(A'')	1629.4828(A'')	1624.4963(A'')	1632.2048(A')
(876.5276)	(837.8386)	1654.0914(A')	1651.5374(A')	1653.1013(A')
895.1104(A'')	873.5819(A')	1660.2728(A'')	1660.1720(A'')	1655.1093(A'')
(899.4025)	(875.0481)	1679.8018(A')	1669.5817(A')	1719.7120(A')
908.7049(A')	880.2369(A'')	3140.7236(A')	3102.7934(A')	3080.5348(A')
(919.5579)	(887.9252)	3176.6805(A'')	3175.6148(A'')	3176.5166(A'')
916.0062(A'')	886.5027(A')	3197.2661(A')	3196.3365(A')	3198.3474(A')
(926.6075)	(893.5094)	3202.1357(A'')	3205.2820(A'')	3208.6167(A'')
943.9950(A'')	901.9306(A'')	3202.8189(A')	3205.5839(A')	3209.6740(A')
(944.4188)	(901.1789)	3206.8256(A'')	3219.0833(A'')	3222.1822(A'')
953.0152(A'')	907.7953(A'')	3207.2759(A')	3219.1546(A')	3222.2690(A')
(962.8473)	(906.7270)	3223.5023(A'')	3234.4206(A'')	3238.7236(A'')
963.2301(A')	912.4546(A')	3223.6169(A')	3234.6136(A')	3238.9028(A')
(963.5189)	(912.6101)	3238.1007(A'')	3246.1289(A'')	3275.5057(A'')
1064.0903(A')	939.3038(A'')	3238.2890(A')	3246.5106(A')	3276.7615(A')
(1045.4830)	(941.4483)			
1072.9897(A'')	1066.0118(A')			
(1064.6964)	(1066.3496)			
1078.5095(A')	1075.6472(A'')			
(1073.7318)	(1076.2947)			
1155.9259(A'')	1156.4228(A'')			
(1156.1739)	(1157.5389)			
1156.5677(A')	1158.7369(A')			
(1157.1987)	(1160.1218)			
1196.9382(A')	1197.1668(A')			
(1197.0194)	(1197.6019)			
1203.6548(A'')	1202.4996(A'')			
(1203.8228)	(1202.8903)			
1215.0033(A')	1214.6177(A')			
(1215.2779)	(1215.0378)			
1248.2866(A')	1241.7505(A')			
(1248.3577)	(1242.2137)			
1275.1930(A'')	1265.3354(A'')			
(1275.0641)	(1265.0224)			
1279.7562(A'')	1275.8784(A'')			
(1280.0424)	(1277.0257)			
1310.6768(A')	1299.9622(A')			
(1310.7085)	(1300.2452)			
1356.0193(A')	1354.8770(A')			
(1356.1918)	(1355.5718)			
1407.1400(A'')	1384.2287(A'')			

(1404.2873)	(1382.9507)			
1444.2713(A'')	1440.3780(A'')			
(1443.8287)	(1441.1161)			
1462.1254(A')	1459.3931(A')			
(1461.9249)	(1460.3781)			
1512.5552(A')	1509.9689(A')			
(1513.4617)	(1511.2062)			
1515.9768(A'')	1512.5639(A'')			
(1516.3855)	(1513.0948)			
1525.0879(A')	1520.9057(A')			
(1524.9136)	(1521.7574)			
1547.0233(A'')	1525.1207(A'')			
(1543.2535)	(1522.8568)			
1555.5046(A')	1562.0341(A'')			
(1556.4796)	(1562.8769)			
1568.4251(A'')	1563.2017(A')			
(1567.0367)	(1564.6022)			
1626.8231(A'')	1615.5601(A'')			
(1623.8883)	(1615.2674)			
1644.3906(A')	1644.0576(A'')			
(1645.0225)	(1645.1520)			
1652.5493(A'')	1649.2689(A')			
(1651.4973)	(1649.9571)			
1668.1223(A')	1668.3477(A')			
(1667.8619)	(1668.9475)			
1706.2522(A'')	1687.9005(A'')			
(1702.9088)	(1688.5890)			
2833.4445(A') ^c	3176.1892(A'')			
(2884.9329)	(3177.6516)			
3168.6706(A'')	3178.3214(A')			
(3172.0400)	(3197.1829)			
3172.6986(A')	3196.3109(A')			
(3175.6487)	(3201.5023)			
3175.8258(A'')	3211.4475(A'')			
(3176.6194)	(3214.1898)			
3195.2491(A')	3212.4712(A')			
(3195.9162)	(3214.4979)			
3213.5432(A'')	3214.7654(A'')			
(3213.8338)	(3222.7900)			
3213.7358(A')	3215.7957(A')			
(3214.0519)	(3224.0119)			
3229.5795(A'')	3230.2164(A'')			
(3229.9722)	(3231.8316)			
3229.6381(A')	3230.3259(A')			
(3230.0288)	(3232.0646)			
3244.0154(A'')	3244.1611(A'')			
(3244.3644)	(3245.7093)			
3244.1116(A')	3244.2725(A')			
(3244.4527)	(3245.8372)			

^aIntermolecular modes; ^bValues in parenthesis have been obtained with BSSE; ^cVery intense C–H stretching mode characteristic of the C⁺–H•••Cl[−] hydrogen bond.

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