Supporting Information

Experimental and Computational Details

In order to select an appropriate density functional for the $[ReCl_x]^+/CH_4$ reaction system, a benchmark for the bond dissociation energy (BDE) of $[Re–Cl]^+$、$[ClRe–Cl]^+$、$[Cl_2Re–Cl]^+$、$[Re–H]^+$、$[Re–CH_2]^+$、$[Re–CH_3]^+$ was carried out. The bond energy of $[M–L]^+$ was calculated with the formulation of $BDE([M–L]^+) = E(M^+) + E(L) − E([M–L]^+)$, where E(X) is composed of the correction to the enthalpy and the single-point energy (SPE). We first optimized the structures of M^+、L、$[M–L]^+$ at B3LYP[1, 2]/cc-PVDZ(pp)[3-6] level and calculated the zero-point vibrational energy (ZPVE) and thermal corrections to the enthalpy. The ZPVE and thermal contribution to enthalpy at 298.15K were corrected with the scaling factors of 0.9689 and 0.9784, respectively, to get the thermal corrections to enthalpy.[7] Then, the SPEs were calculated at CCSD(T)[8, 9]/CBS(aug-cc-pV[T:Q]Z(pp))[10, 11] level of theory using B3LYP/cc-PVDZ(pp). The $BDE([M–L]^+)$ calculated with the thermal correction to enthalpy gained by B3LYP and SPE gained by CCSD(T) acts as the criterion $BDE([M–L]^+)^0$.

Next, the SPE calculations of M^+、L、$[M–L]^+$ were performed by using the methods of B3LYP[1, 2]、B1LYP[12]、B2GP-PLYP[13]、B3P86[14-16]、B3PW91[16, 17]、B98[18]、BPW91[15, 17]、G96LYP[19]、CAM-B3LYP[20]、HCTH93[21]、HISS[22, 23]、HSE03(OHSE2PBE)[24-26]、HSE06(HSEh1PBE)[24-26]、LC-BLYP[27]、LC-ωpbe[28]、M06[29]、M08-HX[30]、M11[31]、mPW1PLYP[32, 33]、mPW1PBE[32, 34]、mPW2PLYP[35]、mPW3PBE[32, 34]、mPWPBE[32, 34]、mPWPW91[17, 32]、OHSE1PBE[25, 26, 36-40]、OLYP[33, 41]、OPBE[34]、PBE0[42]、PBEH1PBE[43]、PKZB[44]、PW91[45]、revTPSS[46]、SOGGA11-X[47]、TPSSh[48]、VSXC[49]、X3LYP[50]、ωB97[51]、ωB97X[51]、ωB97X-D[52]、MN15[53]、MN15L[54]、mPW1PW91[12]、O3LYP[55]、PBE0-DH[56]、Mpw-QIDH[57] with the cc-PVDZ(pp) basis set and the ECP 60 pseudopotential[58] for Re atom. Besides, the methods of B2GP-PLYP, B3PW91, CAM-B3LYP, LC-ωpbe and PBE0 are performed with DFT-D3 dispersion correction.[59, 60] Once again, getting the energy of each elementary by combining the thermal correction to enthalpy gained by B3LYP with

SPE gained by each method, the BDE($[M–L]^+$) of these six bonds were obtained. Taking BDE($[M–L]^+$)^0 as the benchmark, the average errors MSE and variances RMSE of six bonds' BDE for all computational methods are shown in Figure S1. Besides, Figure S2 demonstrates the normal distribution of BDE errors calculated by 15 methods with the small average errors.

Above the analysis, considering the accuracy and precision of the computational method, PBE0-D3(BJ) is employed to optimize the structures. Natural bond orbital (NBO)[61-66] and quasi-restricted orbital (QRO)[67, 68] calculations were performed to obtain further information and the NBOs diagrams were painted by using Multifwn[69] and VMD[70] programs, respectively. The minimum energy crossing points (MECPs) were identified by means of the algorithm developed by Harvey et al.2 in ORCA 4.[71]

Deformation energy (ΔE_{def}) required for distorting the reactants to their geometries in TSs, is calculated as ΔE_{def} = E(CH_4 + $[ReCl_x]^+$ at TS geometry) − E(EC); ΔE_{def} and the respective reaction barrier ($\Delta E^{\ddagger}$) were calculated at the CCSD(T)/BSII level. And the NPA charge of Re in the clusters are calculated at PBE0/def2-TZVP[72] level.

Different components of the total interaction energy of the ground state EC structures in $[ReCl_x]^+$ (x = 1 – 3)/CH_4 and $[ReCl_2L]^+$ (L = F, Cl, Br)/CH_4 systems are calculated at the PBE0-D3(BJ)/def2-TZVP level of theory by using GKS-EDA[73] method in GAMESS package and the input files for GAMESS are produced by MOKIT[74]. The ECP 60 pseudopotential for Re atom is modified to cut off the angular momentum, in which the pseudopotential only includes the definition of the part ≥ g, s, d, f and the part ≥ g is not affected by the pseudopotential. The total interaction energy (ΔE^{tot}) is decomposed to electrostatic energy (ΔE^{ele}), exchange energy (ΔE^{ex}), repulsion energy (ΔE^{rep}), polarization energy (ΔE^{pol}), grimme dispersion correction energy (ΔE^{disp}) and electron correlation energy (ΔE^{corr}), and Pauli repulsion energy (ΔE^{pauli}) is defined as the sum of exchange energy and repulsion energy.

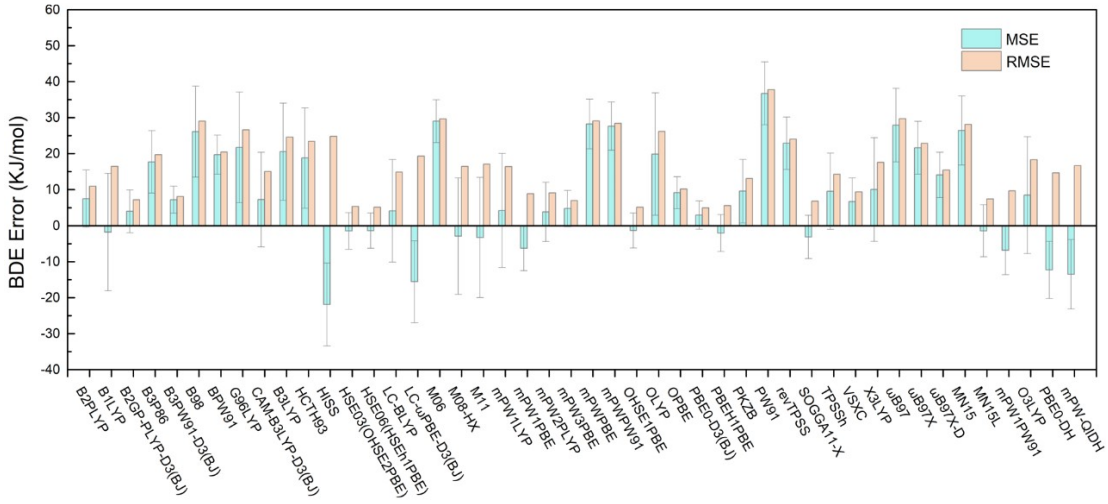


Figure S1. The average errors MSE and variances RMSE of BDE($[Re–Cl]^+$)、BDE ($[ClRe–Cl]^+$)、BDE ($[Cl_2Re–Cl]^+$)、BDE ($[Re–H]^+$)、BDE ($[Re–CH_2]^+$)、BDE ($[Re–CH_3]^+$) for each computational method

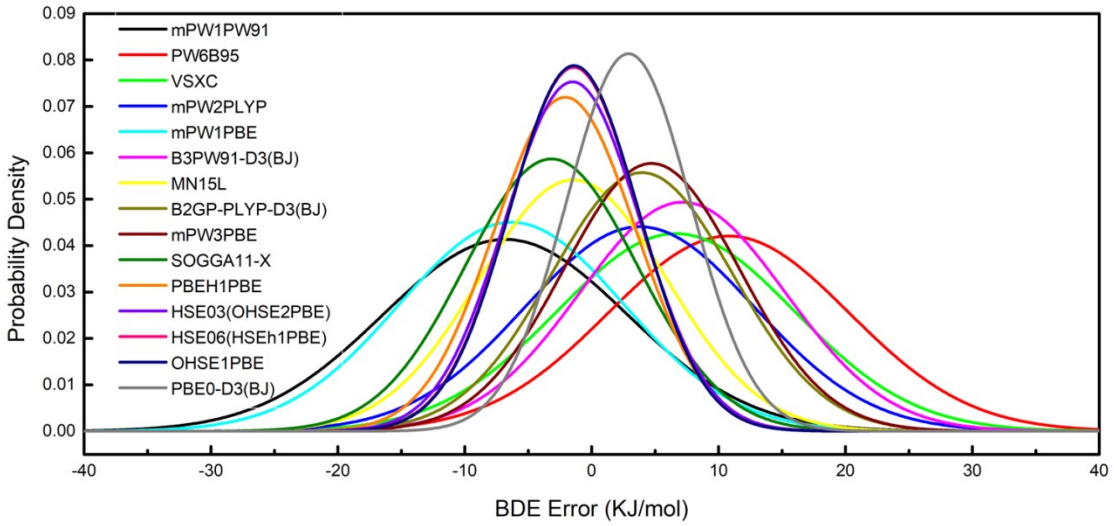


Figure S2. The normal distribution of BDE errors calculated by the methods of mPW1PW91、PW6B95、VSXC、mPW2PLYP、mPW1PBE、B3PW91-D3(BJ)、MN15L、B2GP-PLYP-D3(BJ)、PW3PBE、SOGGA11-X、PBEH1PBE、HSE03(OHSE2PBE)、HSE06(HSEh1PBE)、OHSE1PBE、PBE0-D3(BJ).

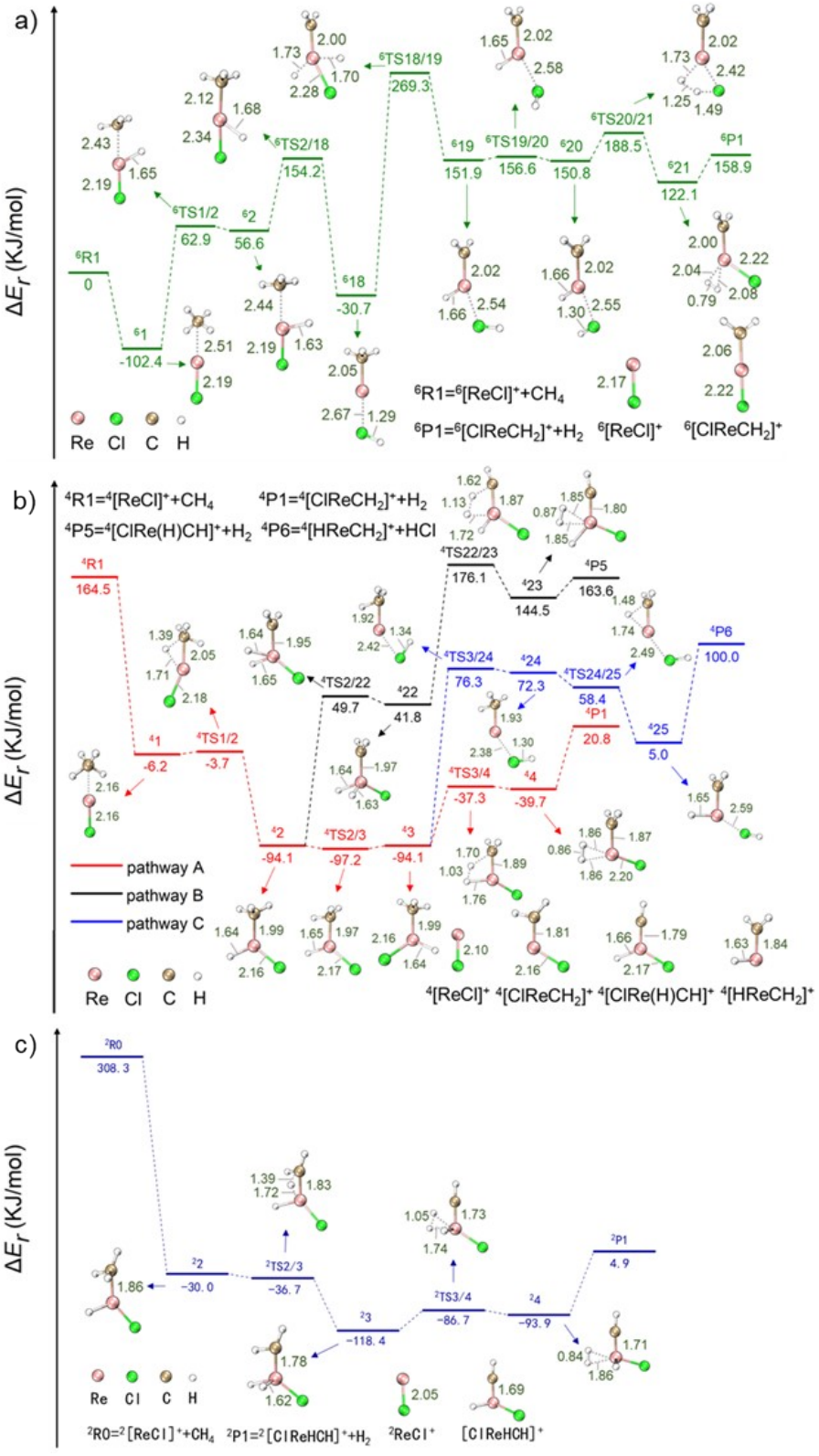


Figure S3. PES and selected structural information for the reaction of a) ^{6}[ReCl]$^{+}$, b) ^{4}[ReCl]$^{+}$ and ^{2}[ReCl]$^{+}$ with CH_4 as calculated at the CCSD(T)/BSII//PBE0-D3(BJ)/BSI level of theory. The relative energies of structures are given in KJ/mol and bond

lengths are given in Å. Charges are omitted for the sake of clarity.

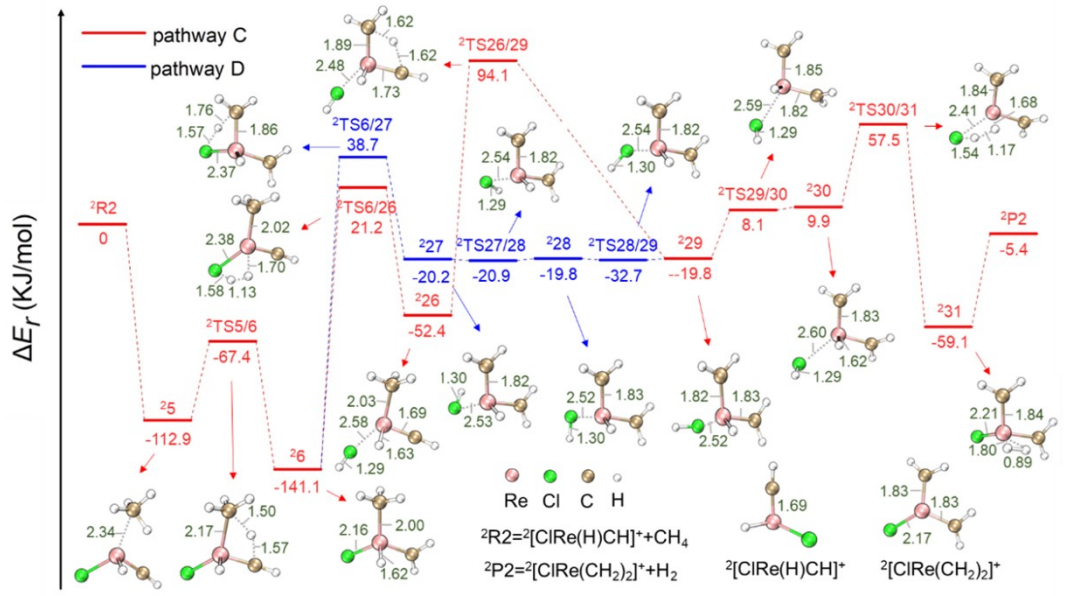


Figure S4. Reaction pathway B and C and selected structural information for the reaction of ^{2}[ClReHCH]$^+$ with CH_4 as calculated at the CCSD(T)/BSII//PBE0-D3(BJ)/BSI level of theory. The relative energies of structures are given in KJ/mol and bond lengths are given in Å. Charges are omitted for the sake of clarity.

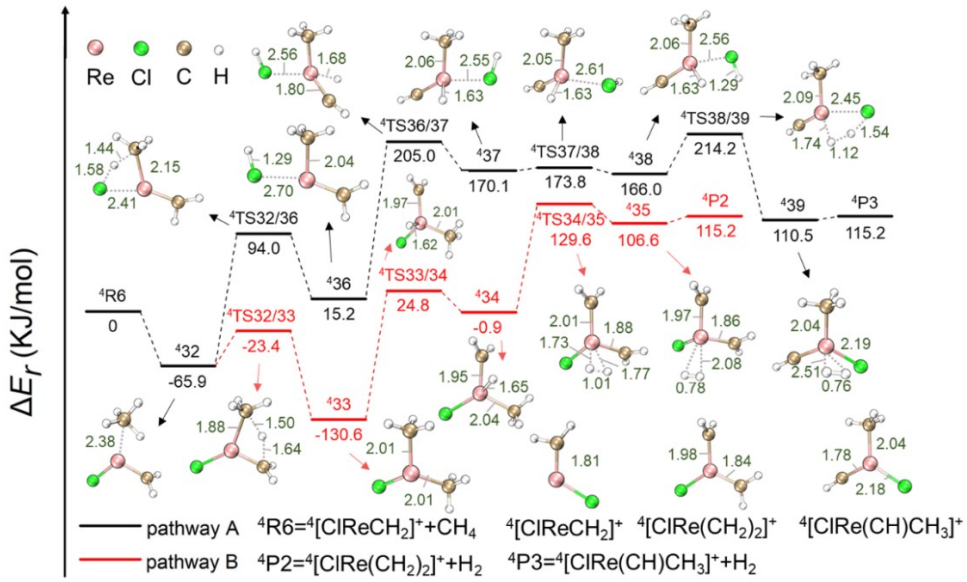


Figure S5. PES and selected structural information for the reaction of ^{4}[ClReCH$_2$]$^+$ with CH_4 as calculated at the CCSD(T)/BSII//PBE0-D3(BJ)/BSI level of theory. The relative energies of structures are given in KJ/mol and bond lengths are given in Å. Charges are omitted for the sake of clarity.

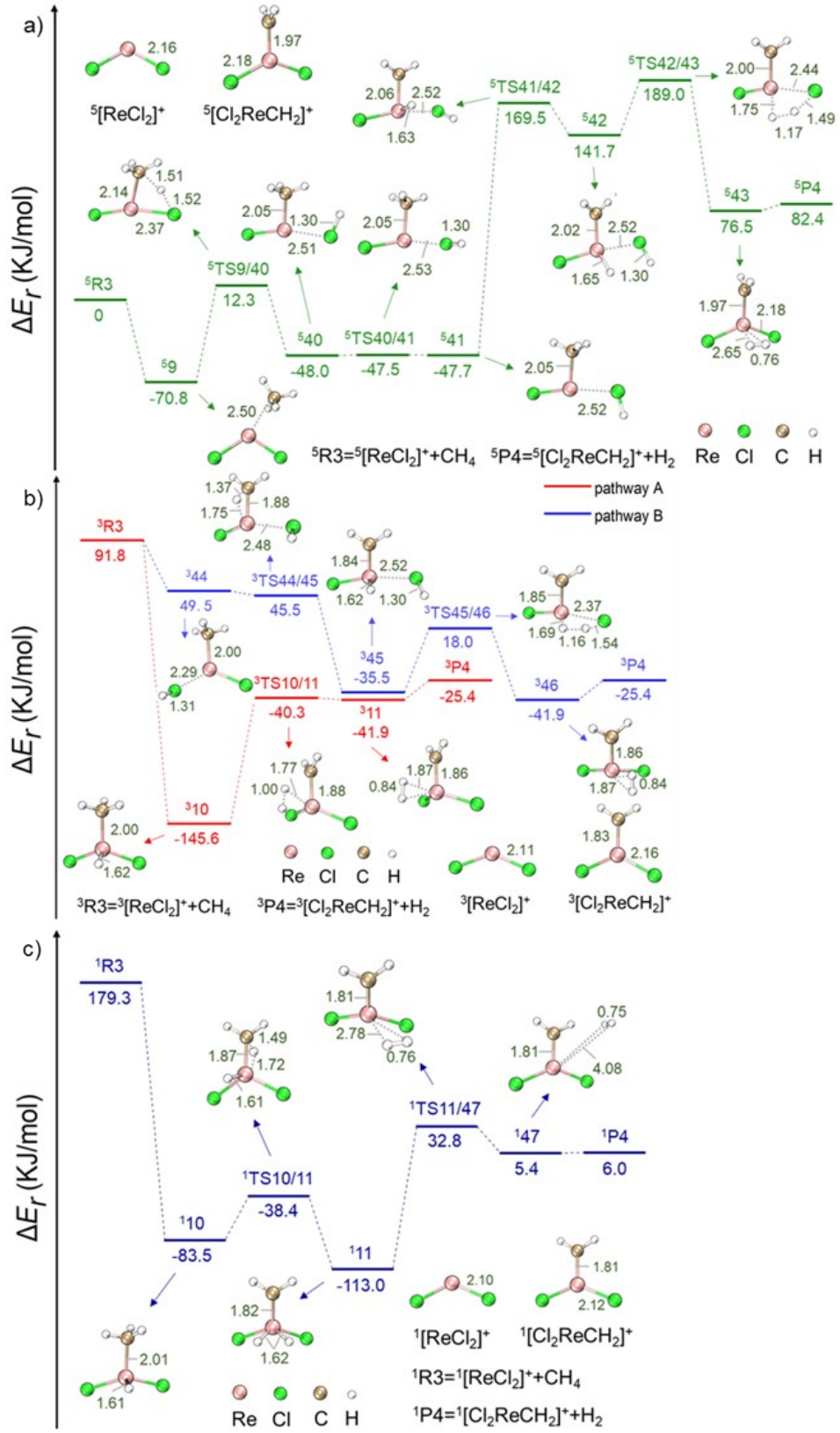


Figure S6. PES and selected structural information for the reaction of a) ^{5}[ReCl$_2$]$^+$, b) ^{3}[ReCl$_2$]$^+$ and ^{1}[ReCl$_2$]$^+$ with CH_4 as calculated at the CCSD(T)/BSII//PBE0-D3(BJ)/BSI level of theory. The relative energies of structures are given in KJ/mol

and bond lengths are given in Å. Charges are omitted for the sake of clarity.

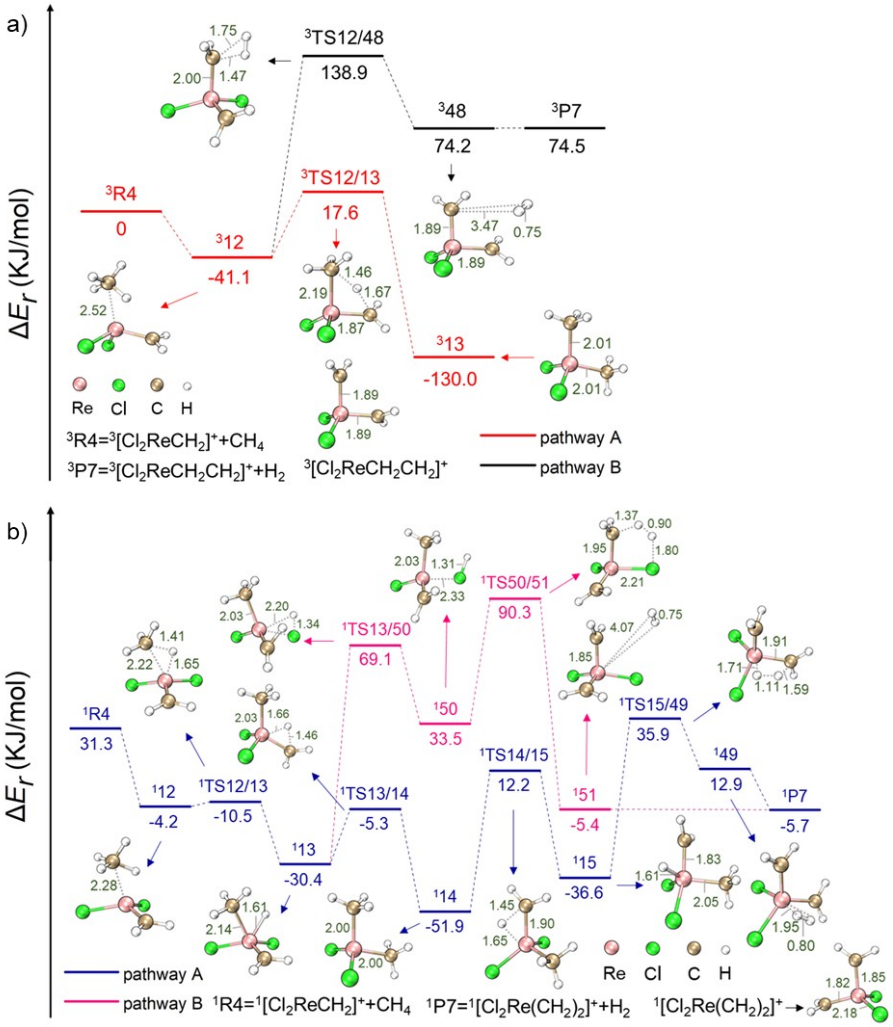


Figure S7. PES and selected structural information for the reaction of a) $^{3}[ReCl_2CH_2]^+$ and b) $^{1}[ReCl_2CH_2]^+$ with CH_4 as calculated at the CCSD(T)/BSII//PBE0-D3(BJ)/BSI level of theory. The relative energies of structures are given in KJ/mol and bond lengths are given in Å. Charges are omitted for the sake of clarity.

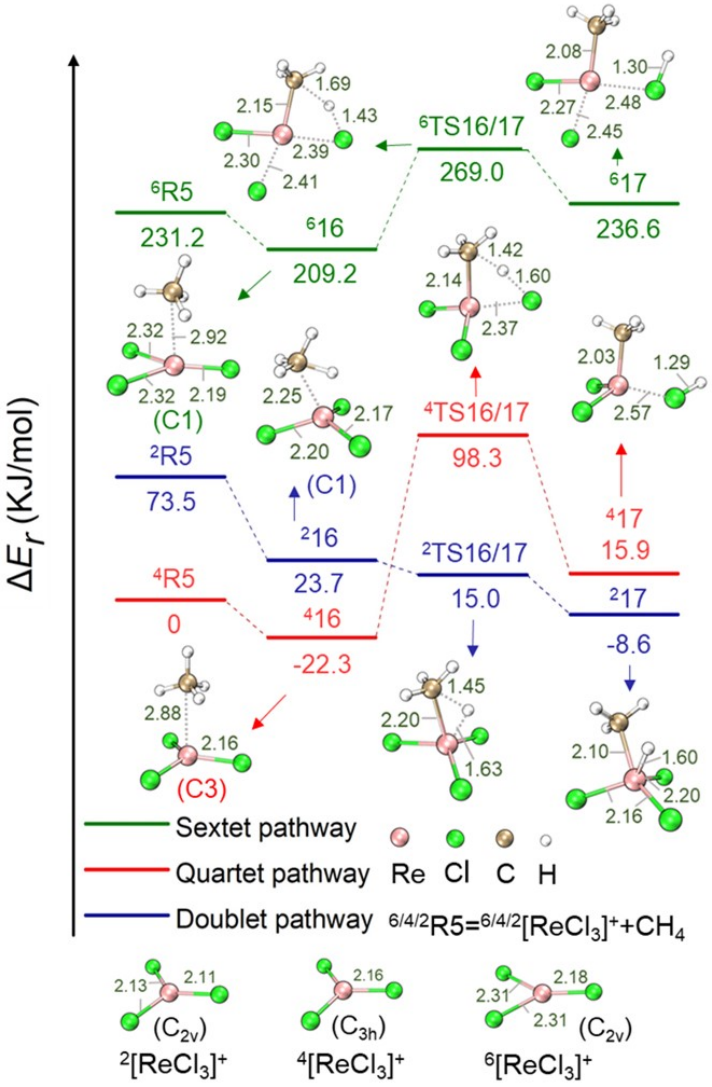


Figure S8. PES and selected structural information for the reaction of $[ReCl_3]^+$ with CH_4 as calculated at the CCSD(T)/BSII//PBE0-D3(BJ)/BSI level of theory. The relative energies of structures are given in KJ/mol and bond lengths are given in Å. Charges are omitted for the sake of clarity.

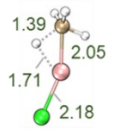
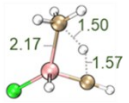
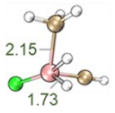
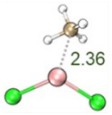
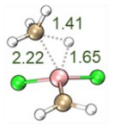
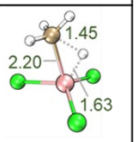
TS	^{4}TS1/2	^{2}TS5/6	^{2}TS5/8	MECP3	^{1}TS12/13	^{2}TS16/17
structure						
ρ_{Me}	-0.01	0.02	0.08	-0.04	-	-0.01
Q_{Me}	0.03	0.02	0.04	0.00	0.08	0.11
Q_H	0.20	0.31	0.24	0.25	0.27	0.27
Q_c	0.77	0.68	0.72	0.65	0.65	0.62
Q_{CT}	0.23	0.32	0.28	0.35	0.35	0.38
ΔE_{def}	371.2	325.6	367.4	211.5	254.9	279.3
$\Delta E^{\ddagger}$	98.7	45.5	65.1	61.5	35.8	37.3

Figure S9. Schematic representations of the TSs together with NPA charges (Q) and spin densities (ρ) on the methyl group (Me), the charge on the transfer–hydrogen (H), cluster (Q_c), the amount of charge transferred (Q_{CT}) from methane to the cluster ion and the deformation energies (KJ/mol) of the reactants in the TSs (ΔE_{def}), the corresponding barriers ($\Delta E^{\ddagger}$).

Table S1. Energy gap (eV) between the electron–donation orbital of methane and the electron-acception orbital of the cluster ($\Delta E_{DO(methane)\rightarrow AO(cluster)}$) for different systems.

System	$\Delta E_{DO(methane)\rightarrow AO(cluster)}$
$^6[ReCl]^+/CH_4$	4.8
$^4[ReCl]^+/CH_4$	1.4
$^5[ReCl_2]^+/CH_4$	0.8
$^3[ReCl_2]^+/CH_4$	0.6
$^4[ReCl_3]^+/CH_4$	5.7
$^2[ReCl_3]^+/CH_4$	0.6

Table S2. Decomposition of interaction energies (KJ/mol) in the ground state EC structures for $[ReCl_x]^+$ (x = 1 – 3)/CH_4 systems as calculated at the PBE0-D3(BJ)/def2-TZVP level of theory.

System	□ΔE^{ele}	□ΔE^{pauli}	□ΔE^{pol}	□ΔE^{disp}	□ΔE^{corr}	□ΔE^{tot}
$[ReCl]^+/CH_4$	-53.2	165.8	-167.9	-6.3	-49.4	-110.5
$[ReCl_2]^+/CH_4$	-80.4	243.6	-195.1	-8.8	-49.8	-90.4
$[ReCl_3]^+/CH_4$	-33.9	82.9	-44.4	-10.9	-28.5	-34.3

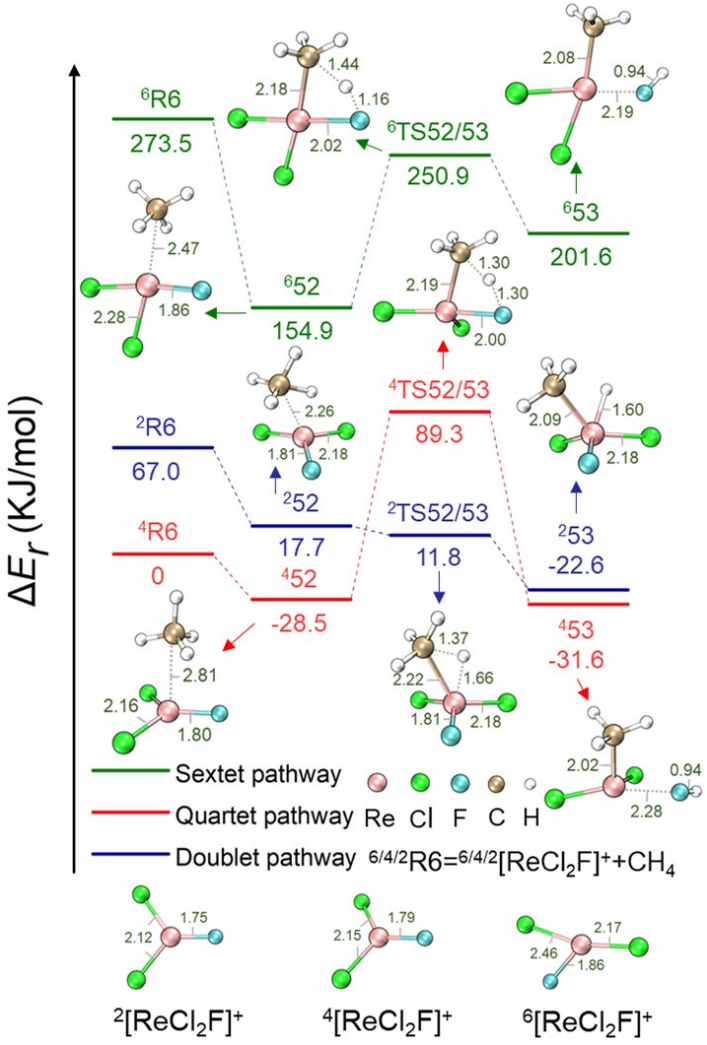


Figure S10. PES and selected structural information for the reaction of $[ReCl_2F]^+$ with CH_4 as calculated at the CCSD(T)/BSII//PBE0-D3(BJ)/BSI level of theory. The relative energies of structures are given in KJ/mol and bond lengths are given in Å. Charges are omitted for the sake of clarity.

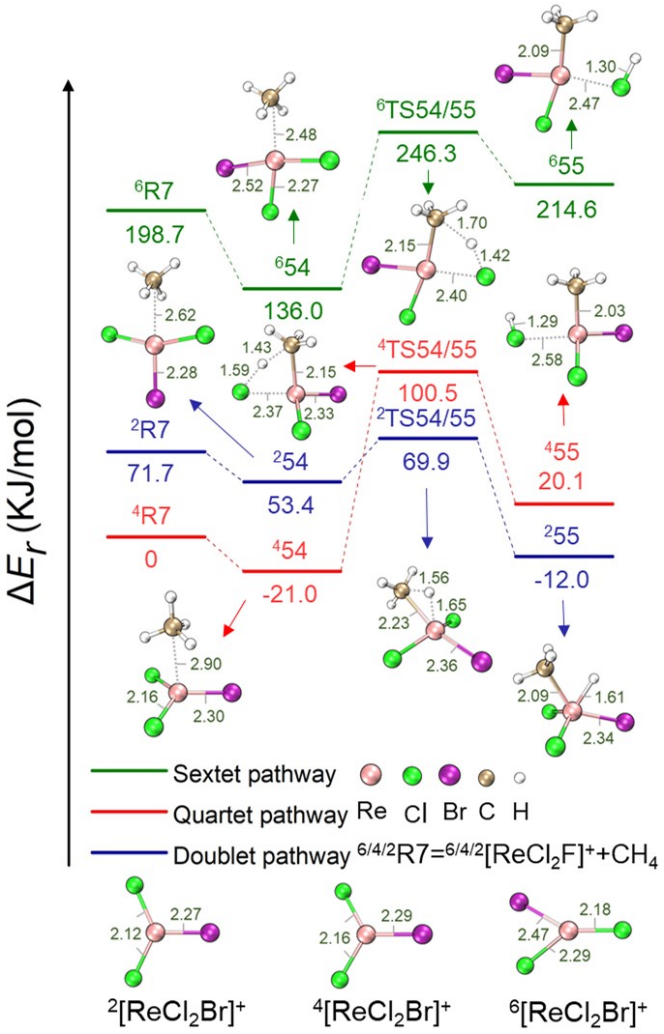


Figure S11. PES and selected structural information for the reaction of $[ReCl_2Br]^+$ with CH_4 as calculated at the CCSD(T)/BSII//PBE0-D3(BJ)/BSI level of theory. The relative energies of structures are given in KJ/mol and bond lengths are given in Å. Charges are omitted for the sake of clarity.

Table S3. NPA charge of Re in $[ReCl_2L]^+$ (*L* = F, Cl, Br) as calculated at the PBE0/def2–TZVP level of theory.

Clusters	Spin state	Charge of Re
	6	1.25
$[ReCl_2F]^+$	4	1.29
	2	1.02
	6	0.93
$[ReCl_3]^+$	4	0.82
	2	0.50
	6	0.84
$[ReCl_2Br]^+$	4	0.69
	2	0.35

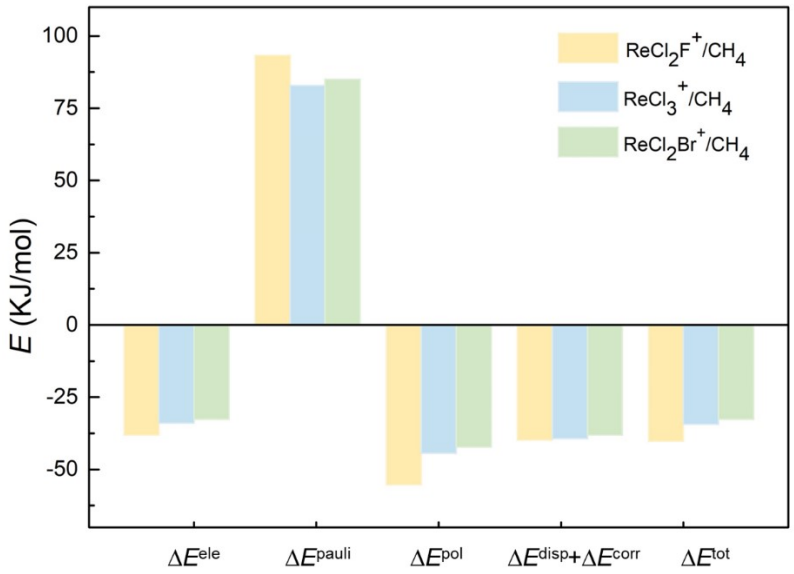


Figure S12. Different components of the total interaction energy of the ground state EC structures in $[ReCl_2L]^+$ (*L* = F, Cl, Br)/CH_4 systems as calculated at the PBE0-D3(BJ)/def2–TZVP level of theory using GKS-EDA method.

Table S4. Decomposition of interaction energies (KJ/mol) in the ground state EC structures for $[ReCl_2L]^+$ (*L* = F, Cl, Br)/CH_4 systems as calculated at the PBE0-D3(BJ)/def2–TZVP level of theory.

System	□ΔE^{ele}	□ΔE^{pauli}	□ΔE^{pol}	□ΔE^{disp}	□ΔE^{corr}	□ΔE^{tot}
$[ReCl_2F]^+/CH_4$	-38.1	93.3	-55.3	-9.6	-30.1	-40.2
$[ReCl_3]^+/CH_4$	-33.9	82.9	-44.4	-10.9	-28.5	-34.3
$[ReCl_2Br]^+/CH_4$	-32.7	85.0	-42.3	-10.9	-27.2	-32.7

Cartesian coordinates

^{6}TS1/2

1 6 (charge multiplicity)

C	2.56381100	-0.05027100	-0.00080100
H	2.88144300	0.41799000	-0.92598100
H	0.97610700	1.41579800	0.00012200
H	2.43397200	-1.13726800	-0.00300200
H	2.88152900	0.41394100	0.92628400
Re	0.13833900	-0.01155000	0.00020500
Cl	-2.05478600	0.00337600	-0.00047000

^{4}TS1/2

1 4

Cl	-1.99057600	0.21728200	0.00012300
Re	0.16452400	-0.10608200	-0.00004900
C	2.15727400	0.39538600	0.00030500
H	1.11358400	1.31864900	-0.00244300
H	2.70935900	0.67287600	-0.89980800
H	2.70698900	0.67365400	0.90163800
H	2.02688400	-0.77510600	0.00036200

^{4}TS2/3

1 4

Cl	1.88923400	0.40424300	-0.00000300
Re	-0.19394100	-0.18921200	0.00000200
C	-1.76804400	0.99814400	-0.00000600
H	-0.61627700	-1.78689300	-0.00005900
H	-2.00340700	1.55281000	0.91155400
H	-2.00340300	1.55281200	-0.91156400
H	-2.34007300	0.01114200	-0.00000800

^{2}TS2/3

1 2

Cl	1.90093200	0.30152400	0.02147300
Re	-0.20274100	-0.13900200	-0.02465700
C	-1.76260300	0.81041400	-0.01217000
H	-0.64948400	-1.52608500	0.70607600
H	-2.41755400	1.66586600	0.11561200
H	-2.21374300	-0.12664500	-0.48220900
H	-1.25384400	0.42364500	1.21781700

^{4}TS3/4

1 4

Cl	1.93198200	0.32804200	-0.00009400
Re	-0.21093100	-0.17617600	0.00006300

C	-1.60286700	1.10045800	-0.00002600
H	-1.42240200	-1.44982900	-0.00134600
H	-2.01599400	1.52362900	0.92123200
H	-2.01469900	1.52438100	-0.92153500
H	-1.95356000	-0.56445700	-0.00128700

^{2}TS3/4

1 2

Cl	1.91910000	0.24793500	-0.00040300
Re	-0.23652100	-0.13848500	-0.01445200
C	-1.44668100	1.09420200	0.01485300
H	-1.46285500	-1.32904900	-0.31485400
H	-2.16546000	1.90947100	0.05076400
H	-1.96091500	-0.40358600	-0.23441400
H	-0.61633900	-0.57055000	1.50016200

^{2}TS5/6

1 2

Cl	2.05927700	-0.26367600	-0.11057600
Re	-0.11437600	0.05661300	0.04842100
C	-0.93457900	1.55050900	-0.21636700
H	-1.39849700	2.51737100	-0.38655700
H	-0.39234800	0.21466100	1.63679700
C	-1.83778500	-1.23704200	-0.16412000
H	-1.56423000	-1.94909000	0.62265000
H	-1.70068900	-1.66546100	-1.16287400
H	-2.90221200	-1.02749500	-0.03065800
H	-1.83731200	0.26574800	-0.14820100

^{2}TS6/7

1 2

Cl	1.99933900	-0.12568400	0.21449700
Re	-0.17797800	0.00147200	-0.14884900
C	-0.82726300	1.58868800	0.50376800
H	-0.38459100	2.53906200	0.18332500
H	-1.58535900	1.66336200	1.28738000
C	-1.27705500	-1.30355200	0.63045400
H	-1.64435700	-0.54494500	-0.97297300
H	-1.21596900	-2.36839000	0.38108800
H	-1.17731900	0.08724600	-1.57463700
H	-2.00689500	-1.06089100	1.40768000

^{2}TS5/8

1 2

Cl	2.00589100	-0.35337000	-0.19435900
Re	-0.13602800	0.07809200	0.13521400

C	-0.62766100	1.55062900	-0.55733700
H	-0.85043700	2.49720500	-1.04288200
H	-1.25386300	0.33926100	1.43135700
C	-1.74595600	-1.21933600	-0.45511100
H	-1.43161900	-2.20364000	-0.09369200
H	-1.56690600	-1.09409700	-1.53202600
H	-2.82270600	-1.10917400	-0.30753600
H	-1.73083500	-0.26689000	0.78247900

^{3}TS10/11

1 3

C	-0.36776100	1.77646300	-0.72265600
H	-1.16228400	1.85535500	-1.46893200
H	-0.97629500	1.42524800	0.90345800
H	-0.78837600	0.72767900	1.59668700
H	0.20471500	2.69454400	-0.55078500
Re	0.01672500	0.16350700	0.16558000
Cl	1.98368400	-0.70687600	-0.25703800
Cl	-1.76754200	-1.03575100	-0.24666900

^{1}TS10/11

1 1

H	-0.57119500	0.48892100	1.51199700
Re	0.01145200	0.19506700	0.03870600
Cl	1.65816300	-1.20836900	-0.06571700
Cl	-1.94811800	-0.75933400	-0.10489200
C	0.46156600	1.97740200	-0.29278300
H	0.78861700	1.36563500	1.03020200
H	-0.34399100	2.71507900	-0.18769500
H	1.42753500	2.38688300	-0.60039500

^{3}TS12/13

1 3

C	0.36810000	1.01685000	-1.62334900
H	-0.07748000	1.98123700	-1.88615700
H	1.04997200	0.59722500	-2.36583000
Re	-0.05073200	0.10086500	-0.04366900
Cl	1.59526100	-1.35648800	0.07075500
Cl	-2.14559300	-0.52166600	0.22130500
C	0.94933400	1.52510200	1.28330900
H	0.24009700	2.33644100	1.45283500
H	1.95974000	1.93302200	1.18191300
H	0.99222100	0.84092200	2.13612700
H	1.09138800	1.42316200	-0.16852500

^{1}TS12/13

1 1

C	-0.07250300	1.57780400	-1.21312000
H	-1.03322300	2.07860900	-1.38591000
H	0.78998200	1.97376900	-1.75392000
Re	-0.05129100	0.15110000	-0.07634700
Cl	1.57179400	-1.32010600	-0.30316400
Cl	-1.99448500	-0.74692000	0.32544400
C	1.22664900	0.99488500	1.53766000
H	0.97649200	1.84871200	2.17343800
H	2.07390800	1.28095500	0.91131600
H	1.45988900	0.12971200	2.15451700
H	-0.15933100	1.05904400	1.30058600

^{1}TS13/14

1 1

C	-0.10225300	0.91329600	-1.75440900
H	0.30710600	1.93010800	-1.66339100
H	-0.55881500	0.70254500	-2.72238500
Re	0.01873600	-0.04558400	-0.12820900
Cl	-1.87639500	0.52216200	0.82475700
Cl	1.95211500	0.38309800	0.75137300
C	-0.21438500	-2.06524600	-0.06210200
H	0.56695600	-2.63820500	-0.56329700
H	-1.15429200	-2.22652100	-0.61525200
H	-0.34518400	-2.36600100	0.98216100
H	0.39160300	-0.46087900	-1.69732800

^{1}TS14/15

1 1

C	0.22958600	1.50904500	-1.43455000
H	0.47601600	0.99667700	-2.36984400
H	0.97980200	2.26518900	-1.17982600
Re	-0.00460300	0.15260100	0.04236000
Cl	1.90923900	-0.90751100	0.13002800
Cl	-1.63384700	-1.27581500	-0.28993800
C	-0.79025300	1.22451700	1.39472100
H	-1.47837500	1.96482900	0.95439700
H	0.59577100	0.81544000	1.43069600
H	-0.79682600	1.22679800	2.48481700
H	-0.74880700	2.00112900	-1.53977300

^{6}TS16/17

1 6

Re	0.10808600	-0.09445900	0.00006200
Cl	-2.00846700	-0.99961700	-0.00015700
Cl	-1.57130200	1.63093300	0.00001500

Cl	2.28627600	0.89937600	-0.00014100
C	1.24632300	-1.91518400	0.00001100
H	2.34937500	-2.01150800	0.00022600
H	0.92789000	-2.45589400	-0.89687100
H	0.92773800	-2.45574300	0.89694100
H	2.20001200	-0.52306400	-0.00023000

^{4}TS16/17

1 4

Re	0.09795300	-0.08303900	-0.08715400
Cl	2.25758300	-0.39894800	-0.34938400
Cl	-0.22006800	2.02131200	0.39823300
Cl	-2.18088900	-0.46404700	-0.61042300
C	-0.38626400	-1.31717000	1.59796800
H	-1.37420400	-1.63677600	1.98476000
H	0.04718900	-0.71505300	2.40081300
H	0.17865300	-2.23215100	1.39979400
H	-1.44320000	-0.97649300	0.71013500

^{2}TS16/17

1 2

Re	0.00066900	-0.07356400	0.02249700
Cl	1.89059600	-1.09540900	-0.21634700
Cl	-0.01842900	1.96222300	-0.81931100
Cl	-1.87148400	-1.12825100	-0.21421600
C	-0.00667000	1.06357100	1.90776300
H	-0.91182400	1.65983100	1.79039900
H	0.88862800	1.67410100	1.78793900
H	-0.00162200	0.60948400	2.90443900
H	0.00309500	-0.36315500	1.63118900

^{6}TS2/18

1 6

C	2.31732600	0.07802600	0.00000400
H	2.64343700	0.58377200	-0.91181400
H	-0.69782000	1.38978400	-0.00000500
H	2.55593500	-0.99868400	0.00007100
H	2.64342400	0.58388300	0.91176600
Re	0.20370300	-0.02837100	-0.00000100
Cl	-2.13686300	0.00593600	0.00000200

^{6}TS18/19

1 6

C	2.14940500	0.47310000	0.00001300
H	2.72341700	0.67524400	0.90827500
H	-0.48058400	-1.68814100	0.00006100

H	-0.24476100	1.52932000	-0.00006600
H	2.72344400	0.67517100	-0.90824800
Re	0.22552400	-0.10872200	0.00000800
Cl	-2.03130900	0.24258700	-0.00004000

^{6}TS19/20

1 6

C	2.21056900	-0.56599200	-0.01286000
H	2.80567800	-0.62320000	-0.92569500
H	-0.10335900	1.69633100	0.08152100
H	-2.55847700	-0.39548800	1.16462300
H	2.80013800	-0.69721700	0.89577700
Re	0.29657200	0.09431300	0.00349800
Cl	-2.26178200	-0.21517300	-0.08243700

^{6}TS20/21

1 6

C	2.16705000	-0.55757100	-0.00009400
H	2.75275100	-0.71334300	-0.90858700
H	-0.47189600	1.67156100	-0.00096400
H	-1.53587100	1.01449500	0.00008600
H	2.75314800	-0.71264700	0.90826200
Re	0.26165300	0.10030200	0.00002900
Cl	-2.12496600	-0.31983900	-0.00002400

^{4}TS2/22

1 4

Cl	-1.88478300	0.38833500	-0.03271200
Re	0.21768700	-0.19280500	0.02800600
C	1.62073000	1.15494800	-0.01516500
H	0.80514700	-1.72311900	-0.19473600
H	1.88434200	1.74773200	-0.89144000
H	2.14686000	1.41996800	0.90887800
H	1.15402000	-0.51556800	-1.27604300

^{4}TS22/23

1 4

Cl	-1.91863200	0.30574200	-0.02266500
Re	0.22921900	-0.13746500	-0.00097800
C	1.62149300	1.10509700	0.01566800
H	1.89395900	-0.39349200	-0.54784600
H	2.53156800	1.60772900	0.34634800
H	1.32671200	-1.36945300	-0.49362800
H	-0.05586100	-1.36309200	1.05977700

^{4}TS3/24

1 4

Cl	-2.13514900	0.23515500	-0.00017700
Re	0.25591900	-0.15780800	0.00004500
C	1.93590000	0.76662800	-0.00019300
H	-1.42021100	1.36631400	0.00201400
H	2.39239800	1.16189200	-0.90968400
H	2.39285300	1.16101400	0.90945800
H	2.12316800	-0.45100700	-0.00096600

^{4}TS24/25

1 4

Cl	-2.18560600	0.18502200	0.07794000
Re	0.28236700	-0.13767300	-0.01789400
C	1.92030500	0.76345200	0.08815400
H	-2.34564900	1.19287200	-0.72142800
H	2.40110500	1.14418800	-0.81794200
H	2.47632200	0.97753900	1.00288200
H	1.92417300	-0.71521600	0.02464900

^{2}TS6/26

1 2

Cl	2.15106400	0.27960100	0.17058500
Re	-0.20211600	-0.02573900	-0.05567700
C	-0.72777700	-1.60665200	0.26729500
H	-0.96115600	-2.64539800	0.48492100
H	0.36870100	-0.52863500	-1.57805100
C	-1.89683700	1.05323800	0.16050200
H	-1.78172100	1.98244900	-0.41496900
H	-1.73610300	1.29424600	1.24065000
H	-2.89807000	0.64644200	0.05825800
H	1.34665500	-0.25143500	-1.08179700

^{2}TS6/27

1 2

Cl	-2.06735900	-0.26911600	-0.18345100
Re	0.26370200	-0.02177000	0.17419200
C	1.40364900	-1.10519300	-0.74957100
H	1.40850400	-2.16966100	-0.47758800
H	1.32346000	0.08815700	1.44129900
C	0.40061800	1.71834100	-0.47039000
H	0.06635400	2.58845400	0.10508300
H	-1.14297800	0.90431800	-0.66597600
H	0.83911000	1.93421700	-1.44759400
H	2.04736200	-0.81664800	-1.58121800

^{2}TS27/28

1 2

Cl	2.23269900	0.09764200	0.16125400
Re	-0.28716200	0.00566500	-0.17486400
C	-0.95901600	-1.50662000	0.59568700
H	-0.86295600	-2.47607700	0.09217000
H	-1.43861600	-0.02198800	-1.34455100
C	-1.10570900	1.39384500	0.67879900
H	-1.06015700	2.39606900	0.23421500
H	2.46955100	-1.10531800	0.57433600
H	-1.64674800	1.31514100	1.62237500
H	-1.49144700	-1.51595300	1.54803000

^{2}TS28/29

1 2

Cl	2.21432900	-0.00008600	-0.26403500
Re	-0.28445200	0.00002500	0.17418800
C	-1.04070500	1.45803300	-0.61851900
H	-0.91737400	2.45604100	-0.18195400
H	-1.43770300	0.00014200	1.34310100
C	-1.04024400	-1.45832000	-0.61819200
H	-1.63165600	-1.40790100	-1.53364000
H	-0.91720000	-2.45609000	-0.18070500
H	-1.63268600	1.40682100	-1.53354000
H	2.71259300	0.00232000	0.93153700

^{2}TS26/29

1 2

Cl	2.24579300	0.10059600	0.09597300
Re	-0.22798500	-0.00875200	0.00725200
C	-1.03842300	-1.53198200	0.01359900
H	-1.62353700	-2.44329500	-0.04207300
H	-0.09304600	0.00132200	-1.62999100
C	-1.66772400	1.21500700	-0.03255400
H	-2.73773900	1.24576600	-0.20139700
H	-1.23034400	2.17415900	0.29764100
H	-1.78572000	-0.24527200	0.65926400
H	2.62763100	0.11545200	-1.14513600

^{2}TS29/30

1 2

Cl	2.33214500	-0.14453000	-0.04744400
Re	-0.26090100	-0.04320000	-0.02896600
C	-0.83035200	1.68271900	0.01291900
H	-0.61770800	2.32874800	-0.85137000
H	-0.11121000	-0.28632700	1.56918500
C	-1.83701800	-1.00844100	0.02151100

H	-1.63724100	-2.08319900	-0.13170500
H	-2.87788500	-0.78823100	0.24218500
H	-1.40952000	2.13519400	0.81936900
H	2.57888200	0.34519400	1.12473300

^{2}TS30/31

1 2

Cl	2.18931700	-0.00006600	0.01721700
Re	-0.21775100	-0.00000700	-0.05739700
C	-1.31798300	1.46737700	0.06789600
H	-0.91670200	2.37773100	-0.40537900
H	0.08128400	-0.00004900	1.59076100
C	-1.31826600	-1.46718400	0.06793900
H	-0.91803100	-2.37756100	-0.40613800
H	-2.24851700	-1.61025100	0.61761700
H	-2.24869000	1.61077300	0.61668600
H	1.18105800	-0.00015700	1.18354400

^{4}TS32/33

1 4

Cl	-2.10254700	-0.19411500	-0.00009200
Re	0.10121700	0.02087300	0.00000700
C	1.06311000	1.63678800	0.00011800
H	1.32720900	2.16580900	-0.92016400
H	1.32718500	2.16569800	0.92047000
C	1.84477500	-1.29633300	0.00000300
H	1.63450300	-1.87527500	0.90521200
H	2.91833800	-1.09070400	-0.00016400
H	1.63427400	-1.87541400	-0.90506700
H	1.86318000	0.20166400	0.00004600

^{4}TS33/34

1 4

Cl	-2.03904800	0.05888500	0.01063600
Re	0.15296100	-0.02677900	-0.00048600
C	1.28373700	1.66663200	0.03034900
H	1.24016300	2.21138800	-0.91762300
H	0.84580400	2.27024300	0.84032200
C	1.16371100	-1.69758700	0.08028400
H	2.32910300	1.44030900	0.26356000
H	1.16636400	-2.45626400	-0.70142700
H	1.74907400	-1.94632800	0.97151300
H	1.17657400	-0.32621500	-1.26450700

^{4}TS34/35

1 4

Cl	-1.98156500	0.26658600	-0.21419500
Re	0.19226500	0.00462800	0.11744900
C	0.72833900	-1.69100000	-0.50722500
H	0.08248200	-2.22025900	-1.21449600
H	1.62079500	-2.23980300	-0.19362300
C	1.56887200	1.38023700	-0.39816700
H	0.02210900	-1.47816300	1.07431800
H	1.87040900	2.16355600	0.30169500
H	2.06642000	1.44580400	-1.36532700
H	-0.17876000	-0.68565600	1.66243200

^{4}TS32/36

1 4

Cl	2.05881500	-0.58028200	0.00003700
Re	-0.30200200	-0.07483200	-0.00002400
C	-2.12942700	-0.41295600	0.00009900
H	-3.12270800	0.02991500	0.00023400
H	-2.16408600	-1.52851900	0.00001800
C	0.46502600	1.93255800	0.00002800
H	-0.00256100	2.32319200	-0.90883900
H	1.49199900	2.34240500	-0.00003400
H	-0.00249400	2.32318000	0.90892900
H	1.43655800	0.86941100	0.00007200

^{4}TS36/37

1 4

Cl	-2.20459320	0.44949599	-0.11037597
Re	0.30940280	0.01019799	0.09333203
C	-0.07512920	-1.97521801	-0.30875597
H	-0.66559720	-2.13045301	-1.21753797
H	-0.60359120	-2.40302201	0.55501403
C	1.58632280	1.02239399	-0.67118097
H	0.89719180	-2.46900401	-0.41786997
H	1.71254980	0.26022099	0.97426003
H	2.48829080	1.27585599	-1.22476097
H	-2.72442520	-0.67657401	-0.48491497

^{4}TS37/38

1 4

Cl	2.25084700	-0.35033900	0.01513300
Re	-0.33943000	-0.06518700	0.02168800
C	-0.05027800	1.96763800	-0.04519500
H	-0.28211700	2.17781600	-1.10589000
H	0.93822400	2.35700000	0.19906900
C	-1.93302300	-0.89466000	-0.20499400
H	-0.82281000	2.41223400	0.59251300

H	-0.28874600	-0.69374100	1.52564700
H	-2.95229700	-1.24110300	-0.36622600
H	2.50040200	-0.60526300	-1.22781900

^{4}TS38/39

1 4

Cl	2.13031100	-0.25053700	-0.19411400
Re	-0.29873600	-0.07639400	0.08423900
C	-0.17893200	2.00760500	-0.08900400
H	-1.13825900	1.93185700	-0.65331800
H	0.63032700	2.41866900	-0.68723400
C	-1.79582700	-0.83864000	-0.47712200
H	-0.30108000	2.48236900	0.88558200
H	0.22279000	-1.35016500	1.15200400
H	-2.58841600	-1.37985300	-0.99076900
H	1.21308000	-1.12800400	0.67247400

^{5}TS9/40

1 5

C	-0.66174300	1.92913400	0.00000000
H	-0.20754500	2.33679800	0.90805800
H	-0.20760900	2.33678700	-0.90809600
H	-1.68906300	0.82180600	0.00001200
H	-1.70670200	2.29304300	0.00003600
Re	0.08936400	-0.07174300	-0.00000100
Cl	-2.22011700	-0.60528500	0.00000100
Cl	2.28359100	-0.21721500	0.00000100

^{5}TS40/41

1 5

C	0.04612800	1.96439500	-0.00239500
H	1.08013600	2.29883600	-0.11070500
H	-0.56049300	2.34180200	-0.83124700
H	2.76963400	-0.19666000	1.18002300
H	-0.37600000	2.32828700	0.94006200
Re	-0.08247400	-0.07865300	-0.00702900
Cl	2.43178800	-0.36814100	-0.05948100
Cl	-2.25558200	-0.37654300	0.02203600

^{5}TS41/42

1 5

C	0.07764200	1.98156400	-0.10301200
H	-0.77854000	2.58435400	0.18306300
H	1.05432800	2.45620900	-0.14127100
H	2.72174700	-0.57322200	1.11355400
Re	-0.08561500	-0.06644800	0.01403700

Cl	2.41461900	-0.34140700	-0.12411800
Cl	-2.24855100	-0.35535300	-0.05982400
H	0.13457500	0.47179800	1.53696500

^{5}TS42/43

1 5

C	0.28857000	1.91998400	0.04674500
H	-0.09114600	2.56278900	0.84240400
H	1.02663400	2.37033700	-0.61788000
H	1.39110400	-1.17054900	0.71177600
Re	-0.07801200	-0.04066300	0.01625000
Cl	2.33533700	-0.36196200	-0.11019300
Cl	-2.24793500	-0.27865100	-0.09859600
H	0.30704400	-1.34235700	1.11386500

^{3}TS44/45

1 3

C	0.27025100	1.83870300	-0.15979100
H	-0.51835700	2.59347300	-0.14029400
H	0.27139000	1.34511700	1.12102500
H	2.64988800	-0.79571600	1.06498800
H	1.26803300	2.22677200	-0.37262500
Re	-0.09744200	0.00320700	0.05219200
Cl	2.32383600	-0.51165300	-0.15966900
Cl	-2.20526500	-0.46730900	-0.11261000

^{3}TS45/46

1 3

C	0.06086500	1.82324000	-0.18024500
H	-0.77568300	2.48553700	0.05706600
H	0.53255800	0.19172300	1.64866900
H	1.51900900	-0.09167200	1.10004000
H	0.95202700	2.30710500	-0.58917800
Re	-0.05141500	-0.00123500	0.07063600
Cl	2.25089300	-0.46714100	-0.20735900
Cl	-2.17659900	-0.45871200	-0.17104500

^{1}TS11/47

1 1

C	-0.09215900	1.85862000	-0.49186000
H	-1.09599900	2.30347200	-0.45877100
H	1.74634100	1.24770800	1.89660700
H	1.02135800	1.10946200	2.06862200
H	0.71773000	2.48749600	-0.86625000
Re	-0.01526500	0.13324300	0.05806600
Cl	1.87982300	-0.86261200	-0.20552500

Cl	-1.92050600	-0.80168700	-0.03235900

^{3}TS12/48

1 3

C	0.30434200	1.71024900	-0.99343700
H	-0.22722600	2.62488200	-0.73552300
H	0.52091900	1.60655800	-2.05878000
Re	-0.02773300	0.03141800	0.04727500
Cl	1.89687200	-1.04535000	-0.17877500
Cl	-2.10078900	-0.60604600	-0.31408600
C	-0.00091300	0.77038300	1.73219600
H	-0.73664000	0.46133700	2.48108000
H	1.65967000	1.97493500	-0.49431800
H	0.75069400	1.48080900	2.08484800
H	1.75854200	2.68507400	-0.87682800

^{1}TS15/49

1 1

C	0.10079700	1.38560000	1.45568900
H	-0.65034300	1.16861700	2.22054100
H	-0.59543600	1.82429200	0.09782800
Re	0.10234800	0.20536000	-0.04105100
Cl	-2.03749900	-0.42949100	-0.24003000
Cl	0.90724500	-1.84570200	0.26286500
C	1.38200100	1.00206300	-1.09026800
H	2.31247500	0.70016000	-0.56620000
H	-0.67775700	1.43739100	-0.93730200
H	1.49729500	1.59450200	-1.99079700
H	0.75519000	2.22532800	1.67404900

^{1}TS13/50

1 1

C	0.06047100	1.52660500	-1.24389400
H	-0.24687300	2.14639600	-0.31511900
H	0.09116100	2.04216800	-2.19696400
Re	0.15795800	0.19435900	-0.07002200
Cl	0.73413400	-1.92111800	-0.22216100
Cl	-2.19286500	-0.24443700	0.33333500
C	1.49045700	0.90721200	1.27817600
H	1.45980400	1.95532500	1.56336900
H	2.40972000	0.73206900	0.67598900
H	1.50626900	0.26418000	2.16136500
H	-1.57406400	0.49443800	1.26734300

^{1}TS50/51

1 1

C	-0.06260500	1.83219100	-0.74803400
H	-1.06192500	2.28216000	-0.76468400
H	0.75358200	2.42675900	-1.16419400
Re	0.07694700	0.16399100	-0.03628500
Cl	2.00912100	-0.81329200	-0.00459000
Cl	-1.76086600	-0.95924300	-0.53436800
C	-0.66512900	0.34728500	1.76279900
H	-1.89941100	-0.22980400	1.87001300
H	-0.96031900	1.29535000	2.20823100
H	-0.19026000	-0.34346100	2.46840300
H	-2.26664600	-0.67410800	1.17733400

^{6}TS52/53

1 6

Re	0.24860900	-0.05304000	-0.00001900
Cl	-1.86143700	-1.15735500	-0.00000900
Cl	-1.47036200	1.47020300	0.00004900
F	1.79775100	-1.35610700	0.00010000
C	2.06968200	1.14201700	-0.00002200
H	2.00873800	1.75587100	0.90162000
H	2.00881200	1.75574600	-0.90175500
H	3.12758500	0.79080300	0.00004700
H	2.25190600	-0.28997900	0.00006700

^{4}TS52/53

1 4

Re	-0.01121400	-0.05990700	-0.10556900
Cl	1.50737200	1.41025700	0.40134000
Cl	-2.03887900	0.74319800	-0.06641600
F	1.44629900	-1.28479900	-0.72851100
C	-0.37633400	-1.97035100	0.89072100
H	-0.37206700	-1.66364400	1.93818200
H	0.20553000	-2.92253300	0.88246600
H	-1.36436800	-2.24357500	0.51704500
H	0.64888600	-1.90068600	0.09853500

^{2}TS52/53

1 2

Re	-0.02027300	0.14383600	-0.09462200
Cl	-1.99050200	-0.64796700	0.39555300
Cl	1.36056600	-1.53535000	-0.22197500
F	-0.07948900	1.64831700	-1.09054700
C	1.34211700	1.13736600	1.34434700
H	1.96116600	0.37841600	1.81357700
H	1.02518300	1.88137000	2.08338400
H	1.86637300	1.67438400	0.54641200

H	0.03934300	0.73549100	1.45126000

^{6}TS54/55

1 6

Re	-0.36515000	-0.05352600	0.00003400
Cl	0.82254800	2.01906700	0.00030600
Cl	-2.71455900	0.42706200	-0.00035100
Br	2.04912100	-0.47419400	-0.00019700
C	-1.07045700	-2.08623200	0.00052400
H	-2.32847900	-0.93659400	-0.00020400
H	-2.12661500	-2.41972800	0.00050900
H	-0.64530700	-2.55001200	-0.89511000
H	-0.64568600	-2.54920800	0.89676400

^{4}TS54/55

1 4

Re	0.18724700	-0.04737000	-0.04562000
Cl	2.36659100	-0.69209200	-0.72598800
Cl	0.75853100	2.02561500	0.33997700
Br	-2.13967900	-0.16610600	-0.18274200
C	0.66875300	-1.29045800	1.63487900
H	0.35393500	-0.63024700	2.44735200
H	1.65065400	-1.68783400	1.95967500
H	0.01053900	-2.15384700	1.51118800
H	1.69050200	-1.08873600	0.65216400

^{2}TS54/55

1 2

Re	-0.32337400	-0.00008200	0.08243400
Cl	-0.67898700	2.02216600	-0.58850000
Cl	-0.67435300	-2.02316200	-0.58862500
Br	2.03447400	0.00129900	0.13211900
C	-2.42608500	-0.00221400	0.83901000
H	-1.04572700	-0.00116200	1.56523200
H	-2.73282700	-0.89469300	1.38278100
H	-2.73512400	0.88956500	1.38261400
H	-2.87659500	-0.00277700	-0.16026600

MECP1

Cl	1.96854232476555	0.00049894808393	0.00045372836349
Re	-0.19571489175736	-0.00032551772021	-0.00018499735677
C	-2.29217305816218	0.00047774296825	0.00074483546155
H	-1.71109873546328	1.07354590136882	-0.00000462509079
H	-2.91196057663834	0.00076126236746	0.90130929905938
H	-2.91371389811522	0.00095130426531	-0.89861487486178
H	-1.71226916462916	-1.07301564133357	-0.00022436557508

MECP2

Cl	-1.90594009738659	0.01080618904801	-0.13213454275195
Re	0.21928160374776	0.03997680278177	0.10713251644261
C	1.67635765679387	1.15915198653018	-0.28002058586407
H	0.86884766930523	-1.45615564706665	0.04600018745790
H	2.12236991766513	2.05234912103496	-0.70489492532026
H	2.10892338616069	0.81687224106884	0.71212619141210
H	1.70911586371391	0.24223130660289	-1.04722784137633

MECP3

Re	0.18393478279192	0.03604668422349	-0.07616560340119
Cl	0.75760697856150	-2.01769360579709	-0.45138550280784
Cl	-1.89006199698657	0.42152166826786	0.41846558011423
C	2.04645414949012	1.35692400229574	-0.05602290510490
H	1.53934109668534	2.29249987353103	-0.30934670025285
H	1.60094758525629	0.74883869316529	0.86375553317651
H	2.37618091070324	0.80121797071004	-0.94532772248174
H	2.94627531349815	1.59235439360362	0.52419032075778

MECP4

C	-0.27642087958554	1.83032272317001	-0.86732892437538
H	-1.18801161359458	2.09592965131223	-1.40986785218922
H	-1.32493755356004	0.59842887789577	1.48603428047510
H	-0.80707026445462	1.24997353233315	1.53291063134094
H	0.56870018579274	2.52397813647735	-0.97131466723254
Re	-0.07834218368139	0.29191854350107	0.12785351601558
Cl	1.88717910189271	-0.56588848204368	-0.26636313214267
Cl	-1.74165567280926	-1.05718702264590	-0.36336605189181

MECP5

C	-0.12456940016376	1.88008057141923	-0.50450710120633
H	-1.07653218830973	2.42645123468666	-0.47706054589346
H	1.27081274496378	0.57039031239533	1.61447689722268
H	0.65647422207481	1.11222328859409	1.76999669274254
H	0.69265975222464	2.36145260497539	-1.04950871980034
Re	0.00407840736277	0.21999251183882	0.28612824466165
Cl	1.83110220918158	-0.74944014104390	-0.45534982007078
Cl	-1.81489974733409	-0.90910338286563	-0.12815764765595

MECP6

C	0.23718081209684	0.87387385247443	-1.79561004990709
H	-0.62866586853194	1.31156522226943	-2.30975320359143
H	1.18855034037853	0.90552613094565	-2.33522106360713
Re	0.02938526635165	0.18239237519472	-0.11110019933446
Cl	1.64706940800490	-1.24875498403233	0.33085101651383
Cl	-1.94837727486226	-0.64393268466639	0.22473814434001

C	1.13340566385335	1.60982533800719	1.45522205152367
H	0.99735081187438	2.63721742344934	1.80855912893955
H	2.18526196603874	1.34392987537193	1.40875218126868
H	0.56903169359419	0.97126480070923	2.14237301889077
H	0.68341118120163	1.86280965027678	0.41336697496359

MECP7

Re	0.09590461507516	-0.27448802581189	0.05519518340479
Cl	1.73775769280192	-0.48038699500734	-1.33813726524439
Cl	0.35669510120570	1.61189002373020	1.12751226233242
Cl	-1.71349529595841	-1.10674218700277	-0.83070887046005
C	-0.44317434359248	-1.27253022456279	2.17599450467503
H	-0.74608580927270	-2.30823417507742	2.33905433716635
H	0.12125521550311	-0.85943209790818	3.00781956702917
H	0.37891471226456	-1.51028933273220	1.35970313642173
H	-1.34924888802687	-0.68652098562758	1.99522414467493

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