SUPPORTING INFORMATION:

Electron-triggered processes in halogenated carboxylates: Dissociation pathways in CF_3COCl molecule and its clusters

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1 Neutral cluster size

We can discuss the neutral $(CF_3COCl)_N$ cluster size generated in our experiment based on the positive and negative ion mass spectra. The present mass spectra (both positive and negative) show evidence for the cluster ion fragments corresponding to the neutral sizes with $N > 10$ molecules. However, it ought to be mentioned that the perpendicular arrangement of our TOF results in certain mass discrimination. Our previous studies[1,2] demonstrated that a region of about 600 m/z can be measured without any mass discrimination. Thus the present decrease of ion abundances at higher masses could be caused by the mass discrimination. On the other hand, it is possible to center the discrimination-free region essentially around any high mass by applying an appropriate deflection voltage in our TOF, which we have done without any significant increase of the ion signals at the higher masses. Thus the observed cluster ion distribution is governed by the neutral cluster fragmentation upon ionization rather than by the apparatus mass discrimination. The positive ionization can lead to a significant fragmentation as observed, e.g., for water[1] and benzene[2] clusters, however, the negative ion spectra are usually less fragmented due to the low electron energy and they span approximately the same range in the present case. Therefore, we assume that the fragmentation after the ionization is not large for the present $(CF_3COCl)_N$ clusters and we have clusters only slightly larger than $N \geq 10$ in the beam.

2 Positive ion mass spectra

2.1 Mass spectra produced under different expansion conditions

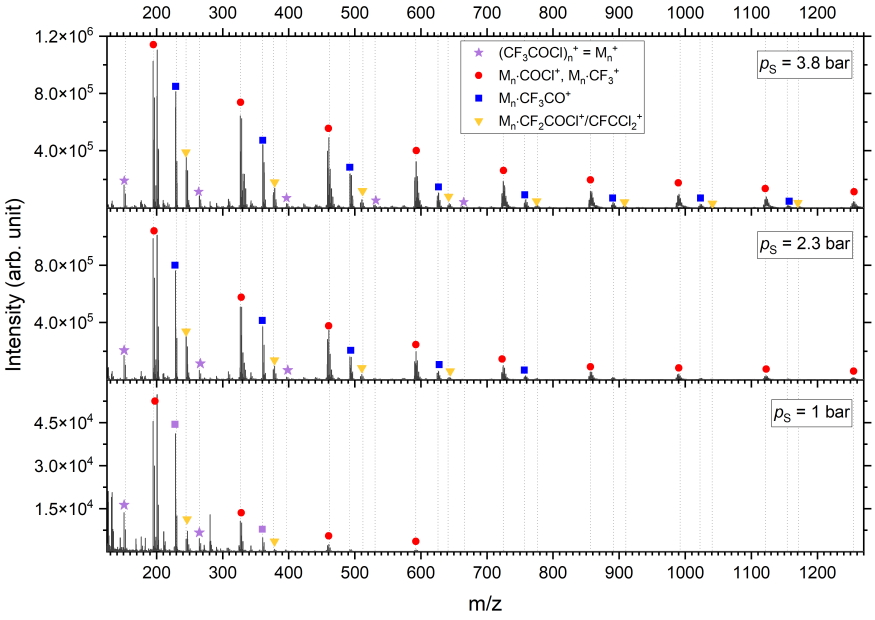

Fig. S1 Comparison of the positive ion mass spectra recorded under different expansion pressure p_S of 5% mixture of CF_3COCl in argon obtained at the ionisation energy of 70 eV.

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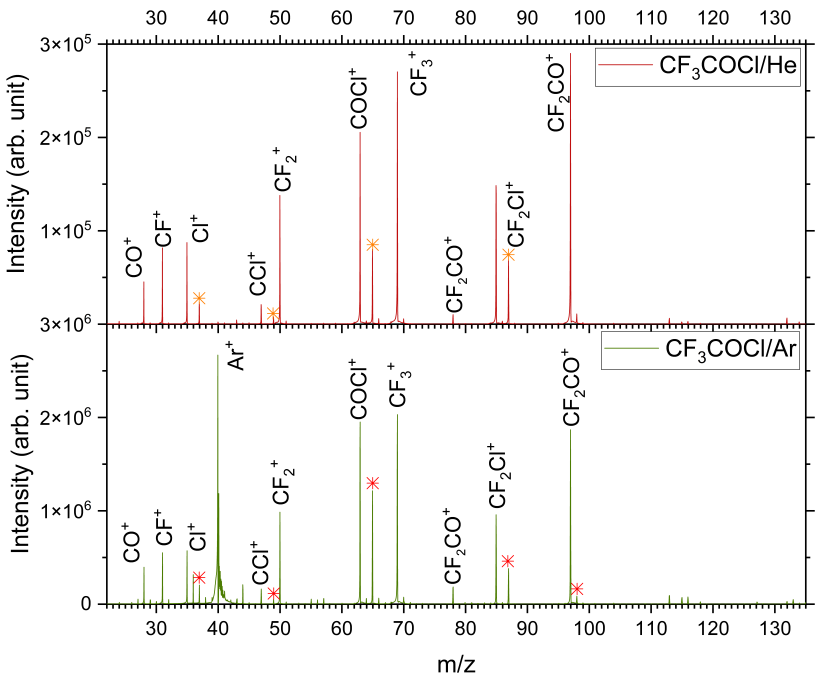

Fig. S2 Comparison of the mass spectra in the m/z range below the molecular mass ($m/z = 132$). Top panel shows the spectrum of isolated molecules produced in co-expansion of 5% CF_3COCl in helium at $p_S = 1$ bar expansion pressure; bottom shows the spectrum of $(CF_3COCl)_N$ clusters produced in argon at $p_S = 3.8$ bar. Orange stars mark isotopic peaks from chlorinated fragments. Positive fragments, electron ionisation, 70 eV electron energy.

2.2 Mass spectra assignment using isotope ratios

Chlorine occurs naturally in two isotopes and the natural ratio of isotopes corresponds to ^{35}Cl :^{37} Cl $= 0.76 : 0.24$. The intensity of a certain fragment containing chlorine atoms is distributed among the mass peaks corresponding to the individual isotopologues. The number and intensity of the mass peaks in an isotopologue multiplet is determined by the number of Cl atoms in the cluster and follows the binomial distribution

$$\mathrm{P} = \binom{n}{k} p^k (1-p)^{n-k}, \tag{1}$$

where P is the normalized intensity (relative abundance) of a specific peak, n is the total number of chlorine atoms in the fragment, k is the number of the ^{35}Cl isotope (i.e., the cluster contains $n-k$ atoms of ^{37}Cl isotopes), and p stands for its relative abundance ($p = 0.76$). For a given n, the relative intensity of each peak in the group can be derived using Eq. 1 and changing k from 0 to n.

Not only chlorine exists in multiple isotopes. Carbon occurs as ^{12}C : ^{13}C $= 0.989 : 0.011$ and oxygen ^{16}O :^{17} O $= 0.998 : 0.002$. Abundances of ^{13}C and ^{17}O are relatively small, yet the cluster ions composed of n CF_3COCl molecules contain n O and $2n$ C atoms. Thus, the isotopic peak of carbon is visible even for 4 carbon atoms (see Fig. S4, first panel, n=1).

For a general case where more than two isotopes exist, the situation is more complicated and multinomial distribution should be applied[3] A web-tool (https://www.sisweb.com/mstools/isotope.htm) can be used to obtain the peak distributions in isotopologue groups.

The first mass peak in the group of peaks corresponding to isotopologues for a given cluster ion size n corresponds to the lightest isotopes, i.e., all Cl atoms in the cluster are ^{35}Cl isotopes. The next mass peak $\Delta m/z = 2$ apart corresponds to the isotopologue with one ^{37}Cl atom. Fig. S3 shows the ratio of intensities of these two mass peaks as a function of the cluster m/z. Vertical dashed lines mark m/z of the clusters composed of n molecules CF_3COCl. Horizontal lines represent the calculated ratios based on the Eq. 1.

The ratios obtained for $(CF_3COCl)_n \cdot COCl^+$ (red dots) are in good agreement with the theoretical ratios for $k = n+1$, i.e., the number of Cl atoms in the cluster is by one larger than the number of CF_3COCl molecules, because of the additional COCl fragment. On the other hand, the ratios for $(CF_3COCl)_n \cdot CF_3CO^+$ (blue squares) are in close to the theoretical ratios for $k = n$, i.e., the number of Cl atoms in the cluster agrees with the number of CF_3COCl molecules, because there is no chlorine in the CF_3CO fragment.

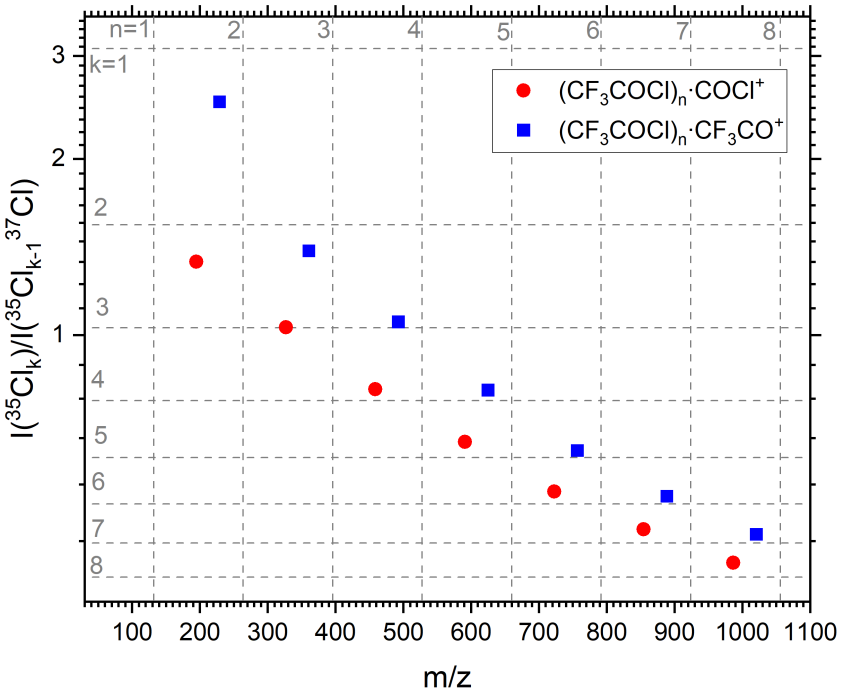

Fig. S3 Plotted intensity (I) ratios of first two peaks of a multiplet (first containing only ^{35}Cl, second having one ^{37}Cl) for the major series. Dashed lines indicate the cluster mass by a number of parent molecules present (n), and the theoretical ratio for particular number of chlorine atoms in the cluster (k). Positive fragments, electron ionisation, 70 eV electron energy.

Fig. S4 illustrates the detailed isotopologue analysis of two mass peak groups of the $M_n{\cdot}CF_3CO^+$ series, which is a standalone series with no significant overlap with any other series up to the high masses.

The analysis becomes more complicated when the series start overlapping, e.g., $(CF_3COCl_n){\cdot}CF_3^+$ and $(CF_3COCl_n){\cdot}COCl^+$, which start to intertwine from $n = 3$, since $m/z = 68$ for CF_3, and $m/z = 63$ for COCl. Nevertheless, Fig. S5 illustrates that we can very well determine the contribution of each individual series.

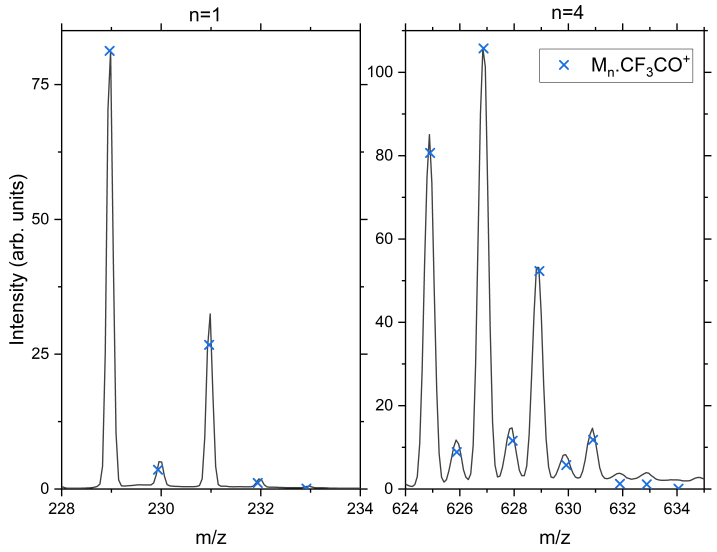

Fig. S4 Isotopic distribution for clusters of $(CF_3COCl)_n{\cdot}CF_3CO^+$ for $n = 1,4$, each containing n chlorine atoms respectively, blue crosses correspond to calculated intensities normalized to the maximum mass peak. Positive fragments, electron ionisation, 70 eV electron energy.

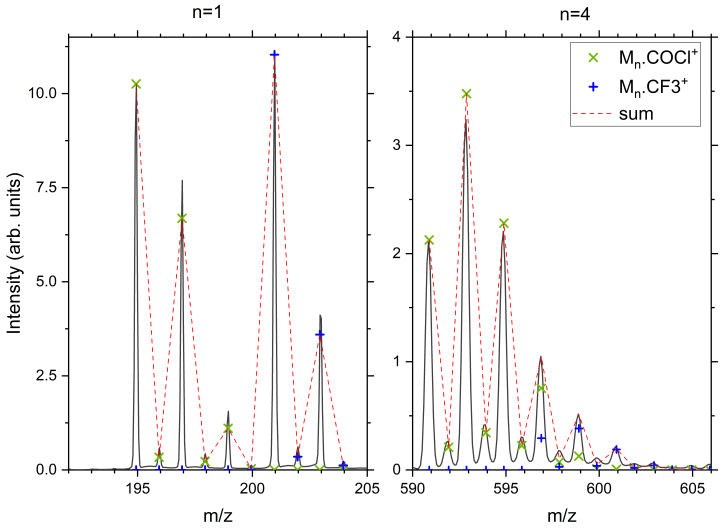

Fig. S5 Isotopic distribution for clusters of $(CF_3COCl_n){\cdot}CF_3^+$ and $(CF_3COCl_n){\cdot}COCl^+$ for $n = 1,4$. Red dashed line is the sum of normalized relative abundances of all fragments contributions (marked with symbols). Positive fragments, electron ionisation, 70 eV electron energy.

2.3 Detailed positive ion mass spectrum

Fig. S6 shows the overall positive spectrum of CF_3COCl clusters in more details. The grey trace shows the mass spectrum 10-times increased in intensity. It exhibits the weak mass peaks not discussed in the main article. For example, the weak M_n^+ series accompanied by a more pronounced protonated $M_n{\cdot}H^+$ ions that most likely originates from water impurities in CF_3COCl sample and/or the argon buffer gas.

One single fragment $CF_3CCl_2^+$ ($m/z = 152$) is recognisable. With higher masses, this area becomes congested and is assignable with difficulties. Further series are labeled by symbols with their putative assignment based on isotopologue ratios given in the top panel. However, it ought to be mentioned that this assignment is ambiguous due to the mass coincidences and spectral congestion in the higher mass regions.

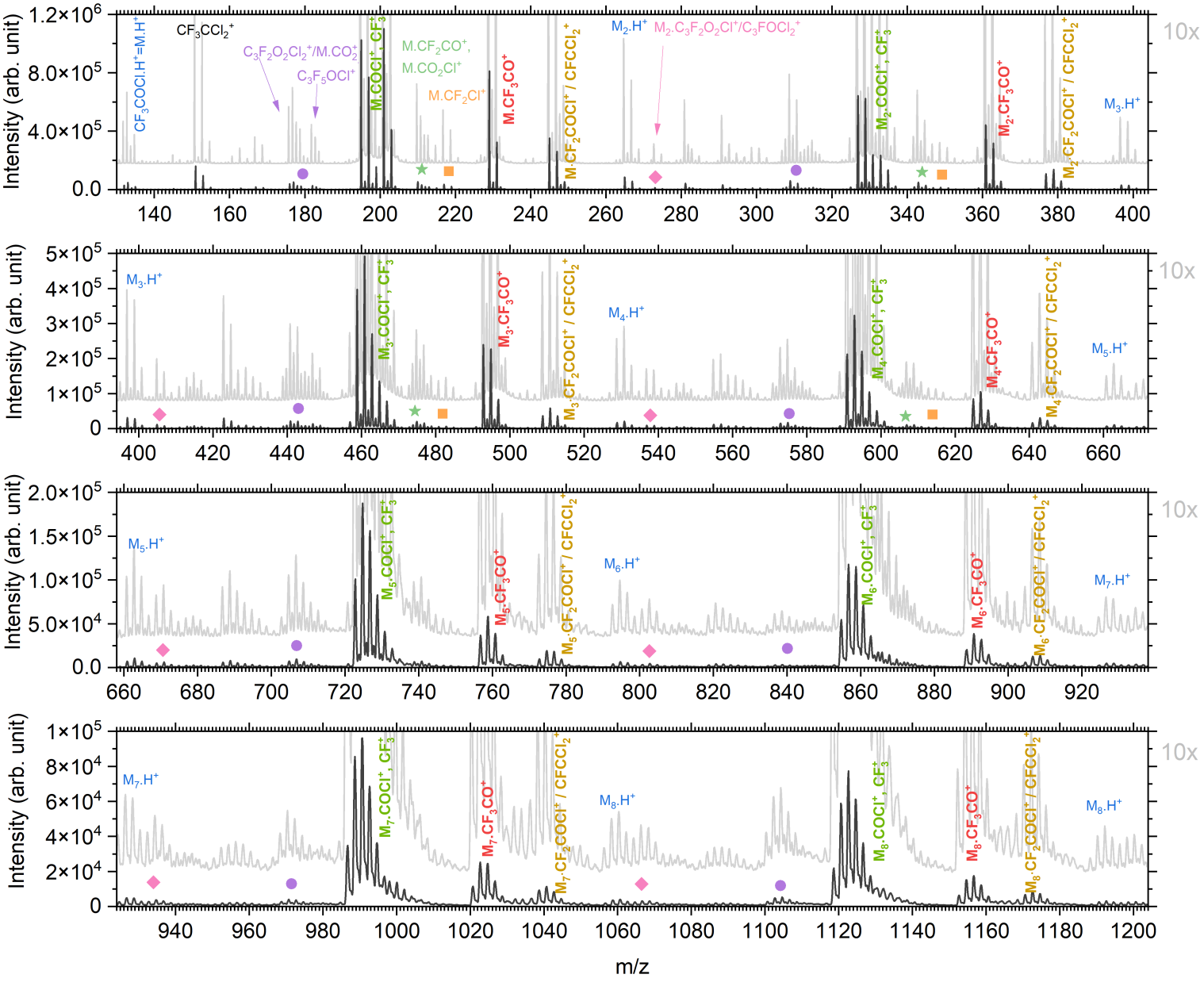

Fig. S6 Detailed mass spectrum of CF_3COCl. The clusters were produced in co-expansion with Ar (5% of CF_3COCl) at 3.8 bar stagnation pressure and ionized with 70 eV electrons. The symbols mark assigned minor series, description is provided above the first point in the top panel. The grey line represents ten times magnified spectrum.

3 Negative ion mass spectra

3.1 Assignment using isotope ratios

To assign the negative cluster ions, the same procedure based on the isotopologue abundances was applied as for the positive spectra above. Fig. 7 shows the graph analogous to Fig. 3 for the positive ions, which supports the unambiguous assignment of the main $(CF_3COCl)_n^-$ and $(CF_3COCl)_n{\cdot}Cl^-$ series.

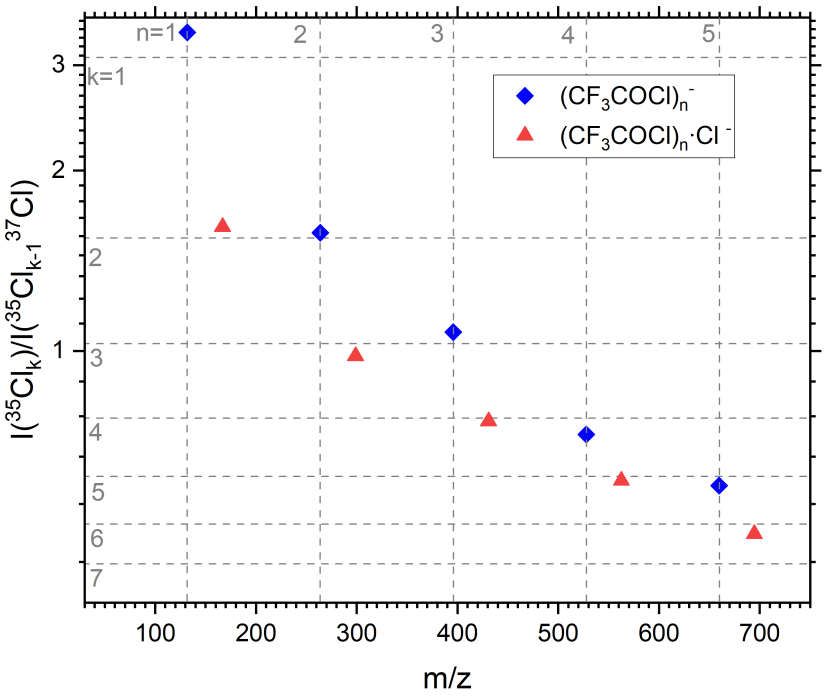

Fig. S7 Plotted intensity ratios of first two peaks of a multiplet for the major series. Dashed lines indicate the cluster mass by a number of parent molecules present (n), and the theoretical ratio for particular number of chlorine atoms in the cluster (k). Ideally, the points should be in between the vertical lines and on the horizontal lines. Negative fragments, electron attachment, 5 eV electron energy.

We have a series with fragments differing in mass by only two units – $(CF_3COCl)_n \cdot CF_3^-$, $(CF_3COCl)_n \cdot Cl_2^-$. In Fig. S8 we have six panels, the first row containing clusters of $n = 1$, second row $n = 2$. Columns show three situations considering different fragments. In the first one, we have only CF_3^- and Cl_2^- and it is obvious that there is another series wedged in between them (our series Y in Section 3.2). Second and third column show the plot with a sum of intensities after introducing series $(CF_3COCl)_n \cdot CO_3Cl_3F_2^-$ and $(CF_3COCl)_n \cdot CO_2Cl_4F^-$, respectively. Both are similarly possible. Due to the low intensity and high congestion of the spectra for higher masses, fits on larger clusters are inconclusive.

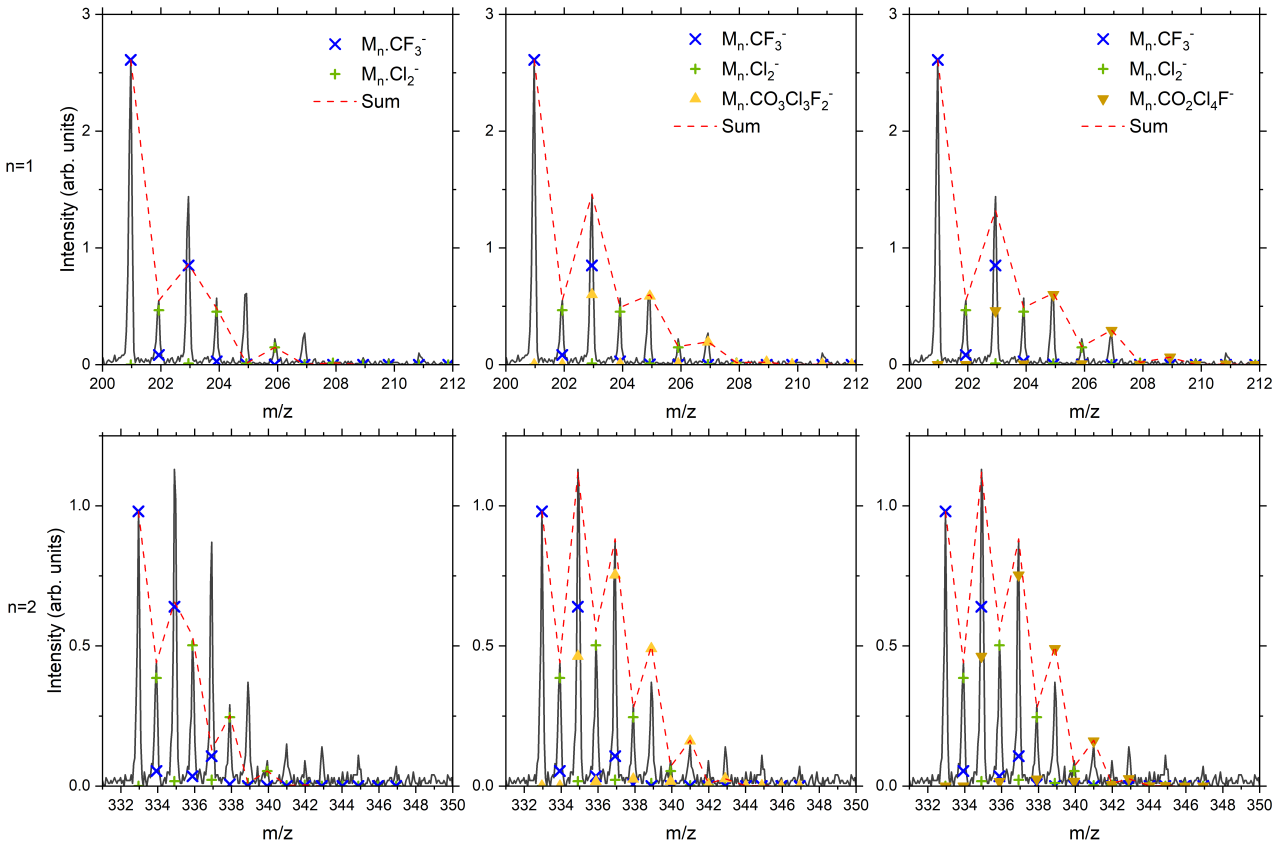

Fig. S8 Comparison of isotopic distributions for clusters of $(CF_3COCl)_n \cdot CF_3^-$, $(CF_3COCl)_n \cdot Cl_2^-$ and $(CF_3COCl)_n \cdot CO_3Cl_3F_2^+$ or $(CF_3COCl)_n \cdot CO_2Cl_4F^+$ for $n = 1, 2$. Red dashed line is the sum of normalized relative abundances of all fragments contributions (symbols). Negative fragments, electron attachment, 5 eV electron energy.

3.2 Detailed negative ion mass spectrum

Fig. S9 contains a negative spectrum of CF_3COCl clusters. Once we zoom in ($10\times$), we see three nonabundant series in between the main ones (M_n^-, $M_n{\cdot}Cl^-$ and $M_n{\cdot}CF3^- + Cl_2^- + Y^-$, Y = $CO_3Cl_3F_2^+$ or $CO_2Cl_4F^+$).

Yellow circles mark a $M_n{\cdot}CF_3CO_2^-/M_n{\cdot}CF_2CCl^-$ series and $M_n{\cdot}CF_2COCl^-$ is enhanced by pink squares. The assignment is with high uncertainty. The intensity of bigger clusters in those series is close to the noise level, so it is difficult to identify the correct peaks for isotopic analysis.

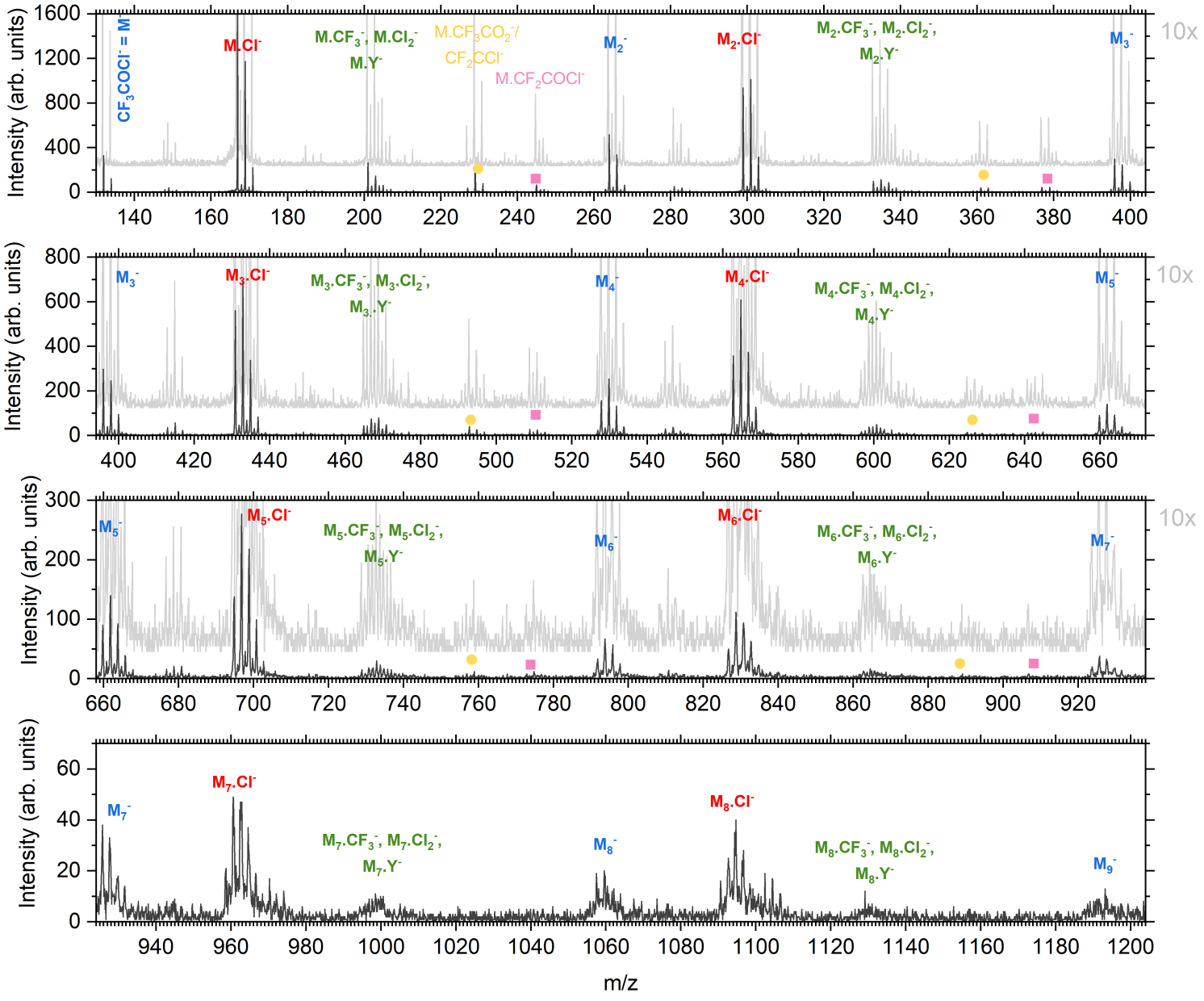

Fig. S9 Detailed look on CF_3COCl clusters. Symbols mark assigned minor series, description is provided always above the first point. Grey line represents ten times magnified spectrum. Negative fragments, electron attachment, 5 eV electron energy, produced in co-expansion with Ar (5% of CF_3COCl) at 3.8 bar (abs) expansion pressure.

4 Theoretical part

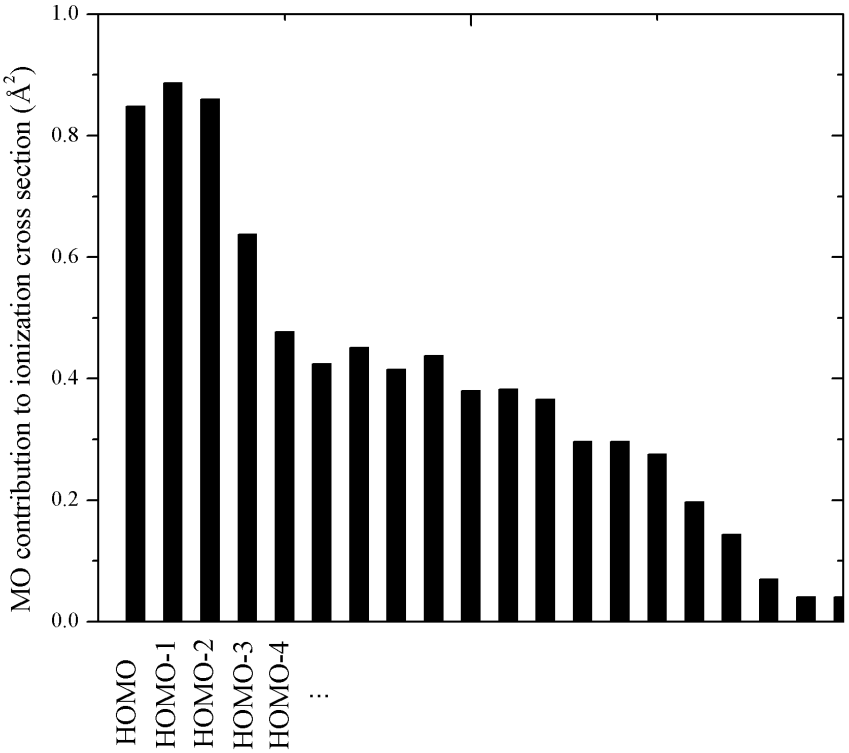

Fig. S10 Calculated ionization cross section contributions of individual molecular orbitals in the BEB formalism.

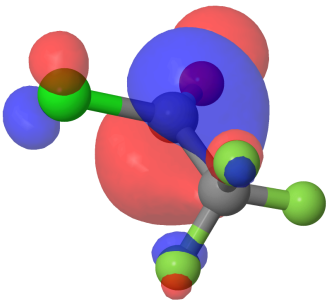

Fig. S11 Isosurface of the LUMO of neutral CF_3COCl molecule (cutoff value 0.05 a.u.).

Figures S12–S20 include structures obtained through genetic algorithm optimization.

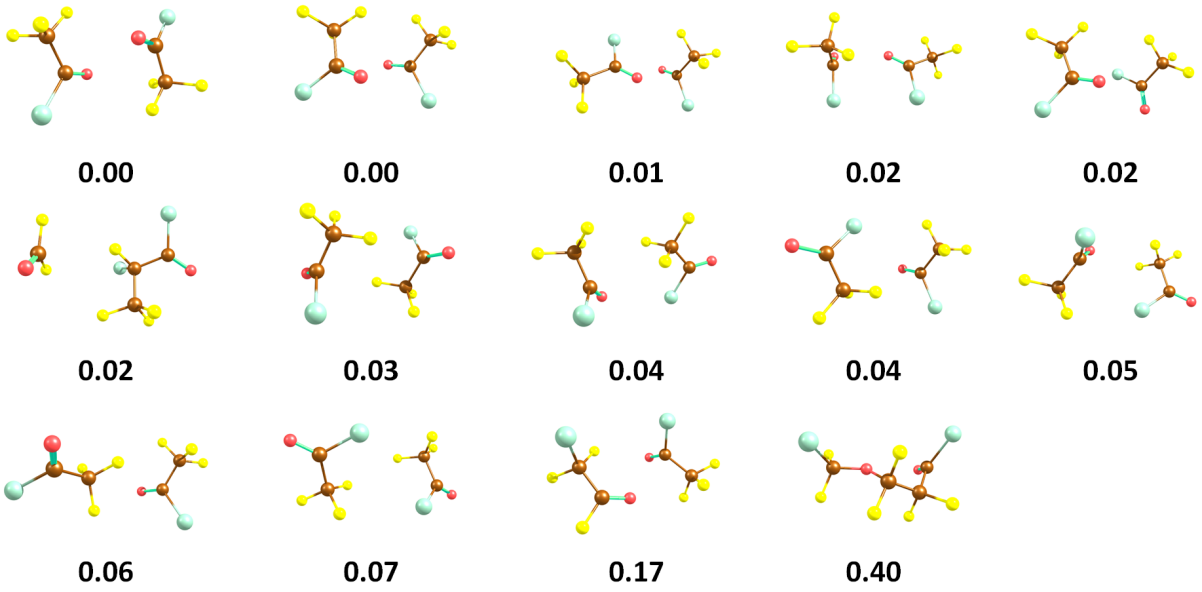

Fig. S12 Selected structures of neutral CF_3COCl dimer clusters obtained through genetic algorithm optimization as optimized at the B3LYP-D3/aug-cc-pVDZ level along with the relative energy (in eV).

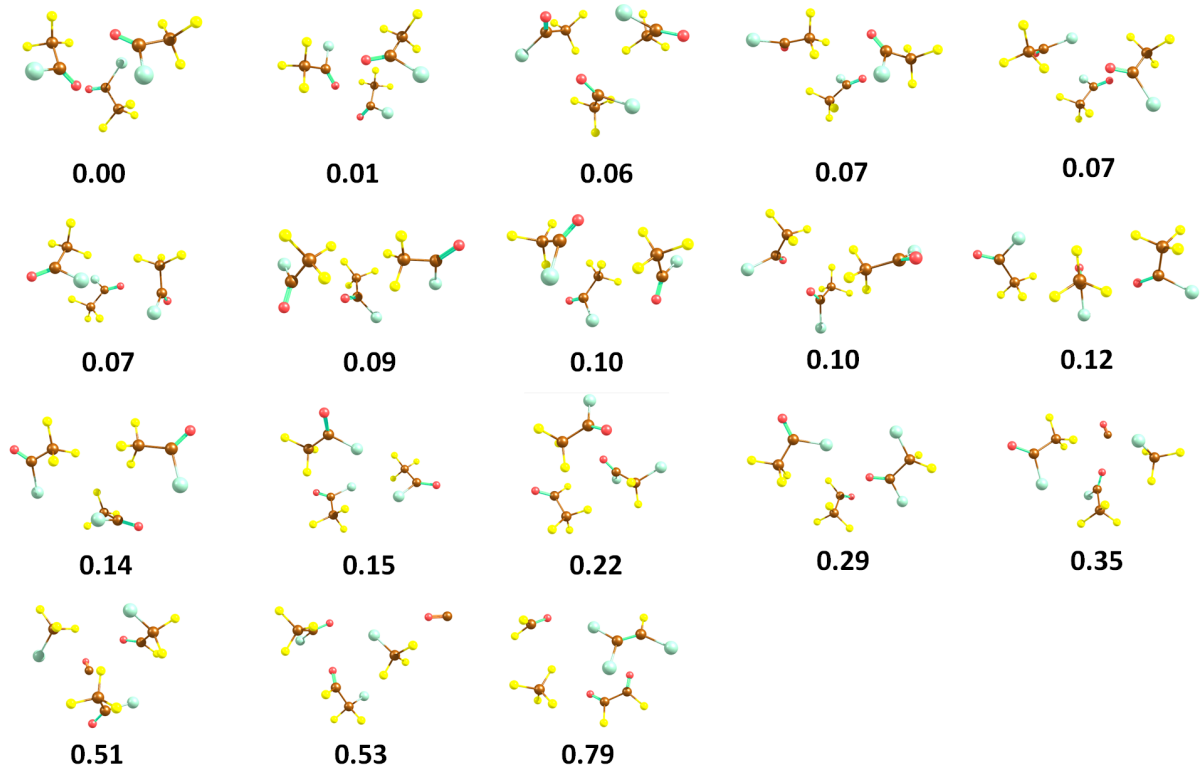

Fig. S13 Selected structures of neutral CF_3COCl trimer clusters obtained through genetic algorithm optimization as optimized at the B3LYP-D3/aug-cc-pVDZ level along with the relative energy (in eV).

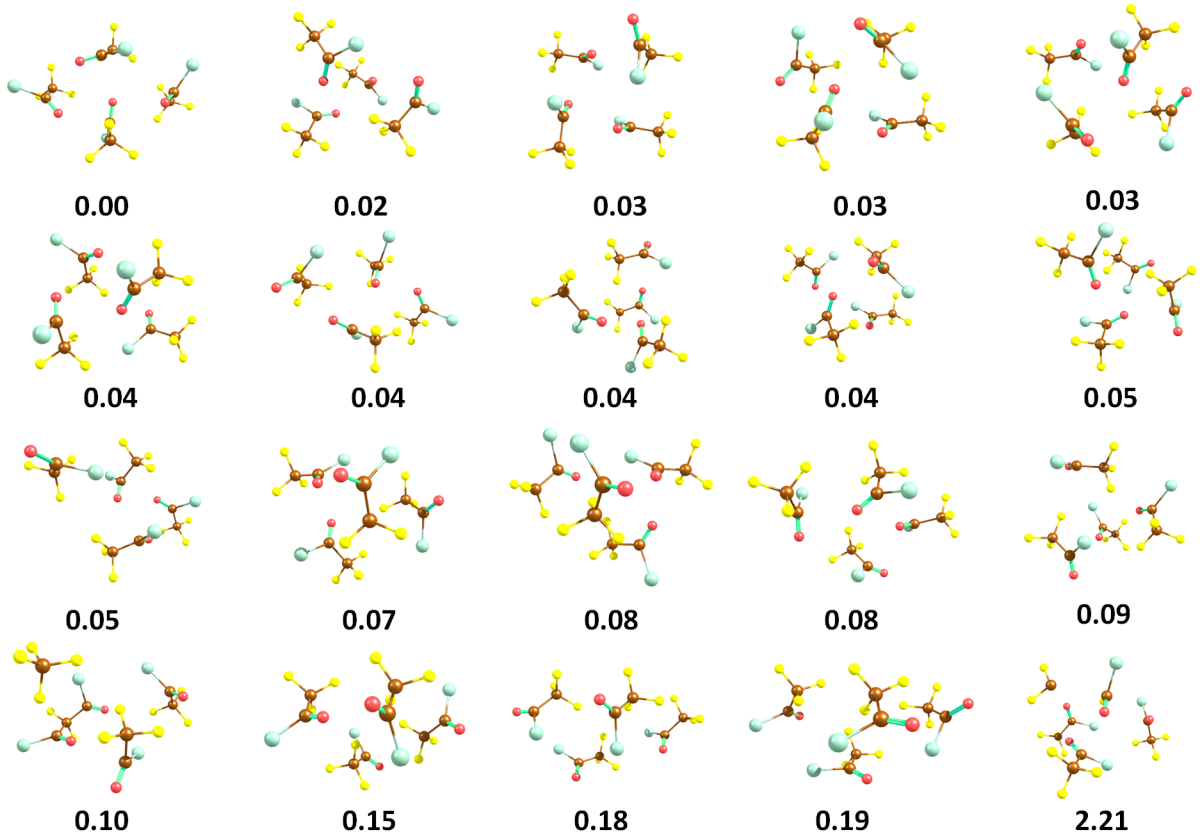

Fig. S14 Selected structures of neutral CF_3COCl tetramer clusters obtained through genetic algorithm optimization as optimized at the B3LYP-D3/aug-cc-pVDZ level along with the relative energy (in eV).

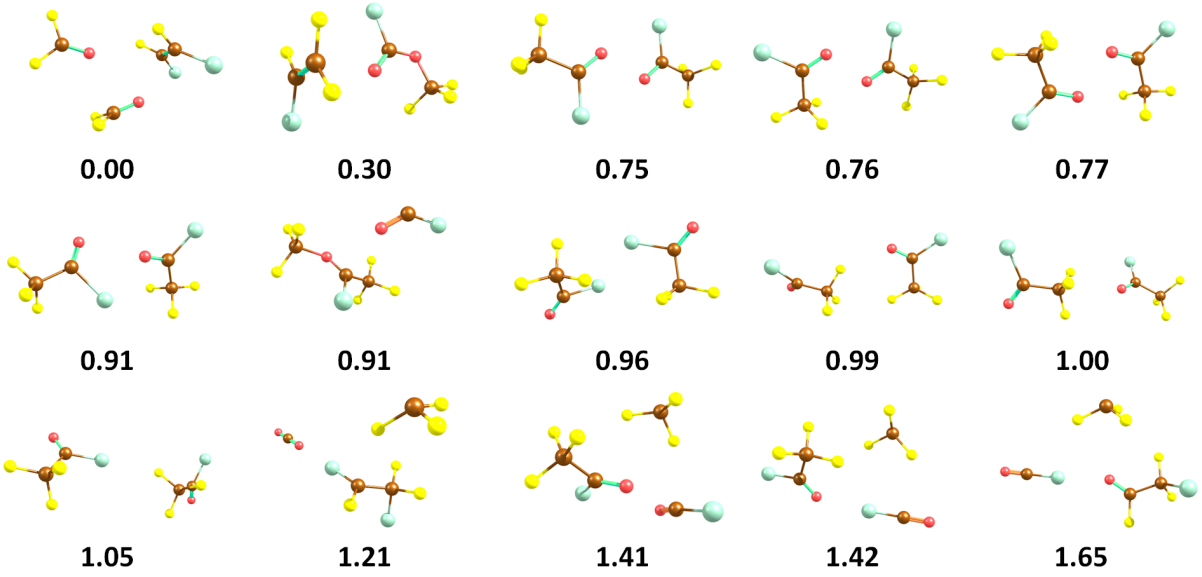

Fig. S15 Selected structures of cationic CF_3COCl dimer clusters obtained through genetic algorithm optimization as optimized at the B3LYP-D3/aug-cc-pVDZ level along with the relative energy (in eV).

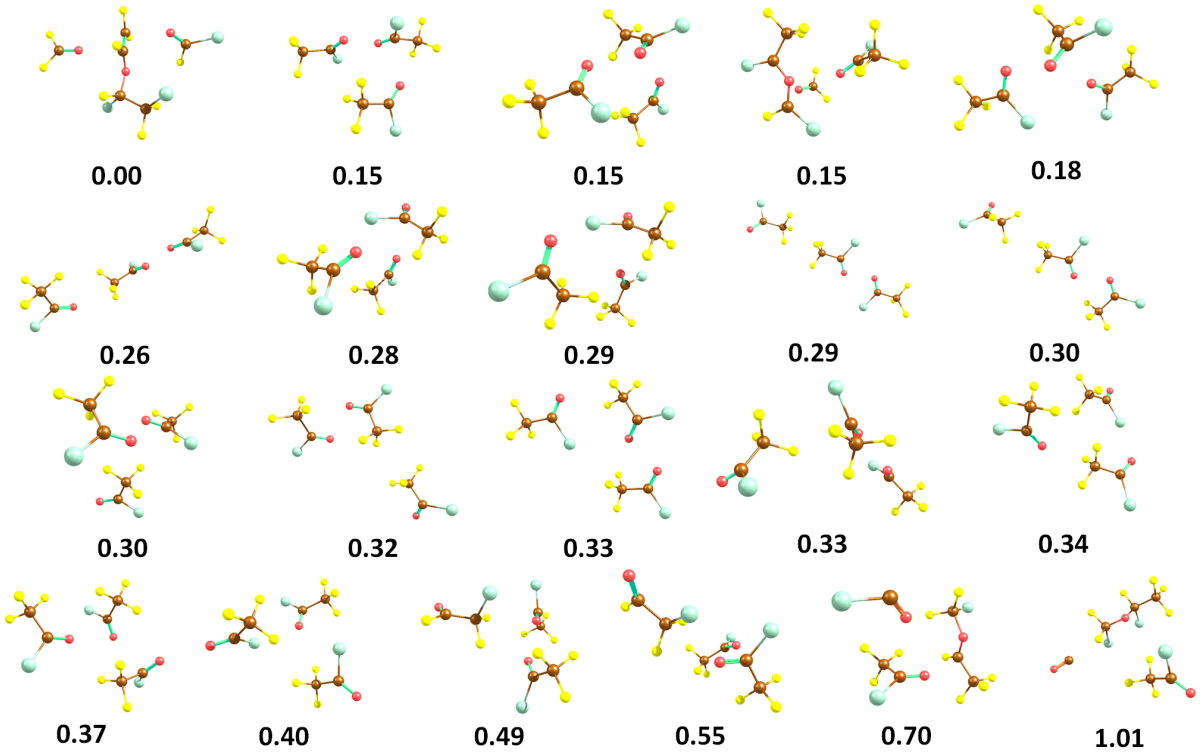

Fig. S16 Selected structures of cationic CF_3COCl trimer clusters obtained through genetic algorithm optimization as optimized at the B3LYP-D3/aug-cc-pVDZ level along with the relative energy (in eV).

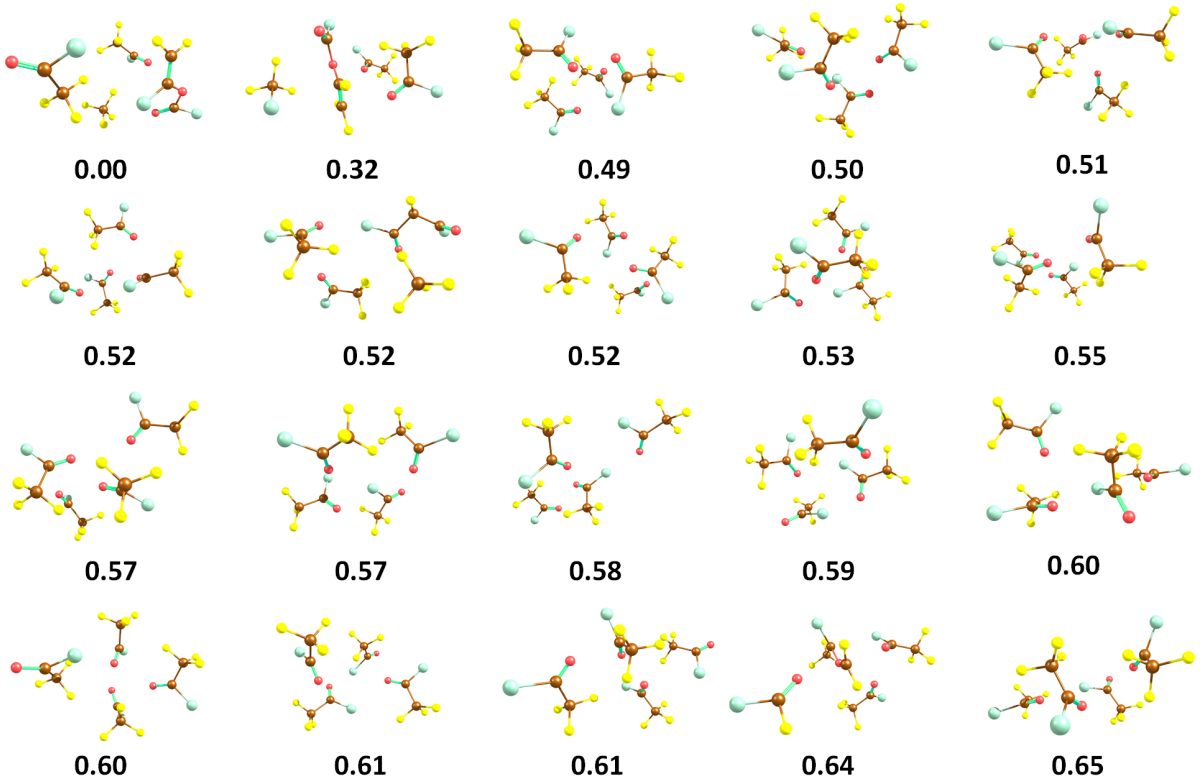

Fig. S17 Selected structures of cationic CF_3COCl tetramer clusters obtained through genetic algorithm optimization as optimized at the B3LYP-D3/aug-cc-pVDZ level along with the relative energy (in eV).

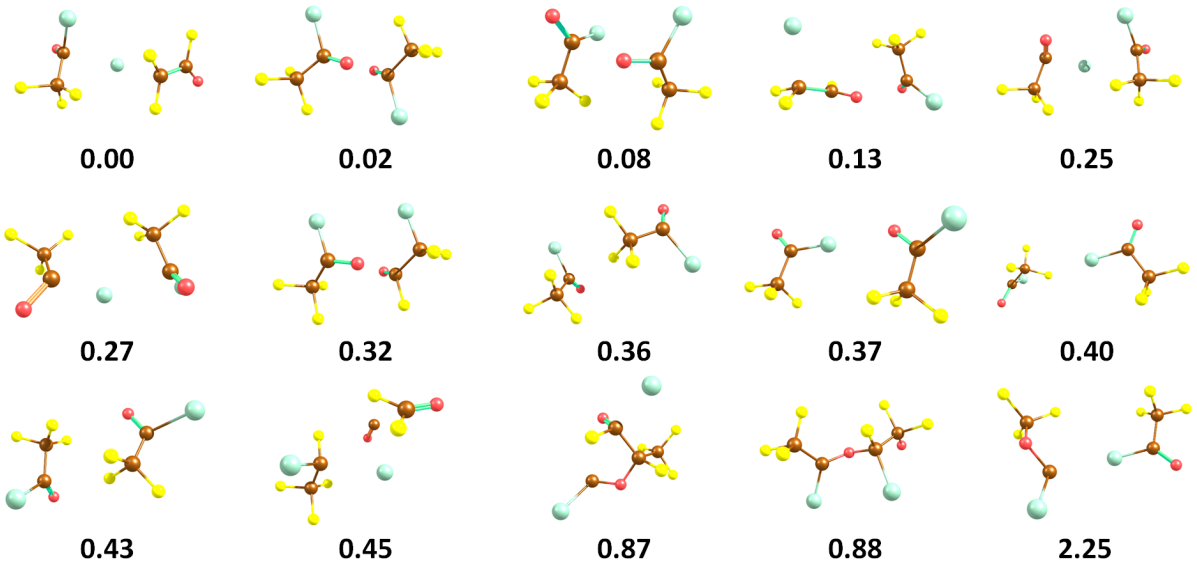

Fig. S18 Selected structures of anionic CF_3COCl dimer clusters obtained through genetic algorithm optimization as optimized at the B3LYP-D3/aug-cc-pVDZ level along with the relative energy (in eV).

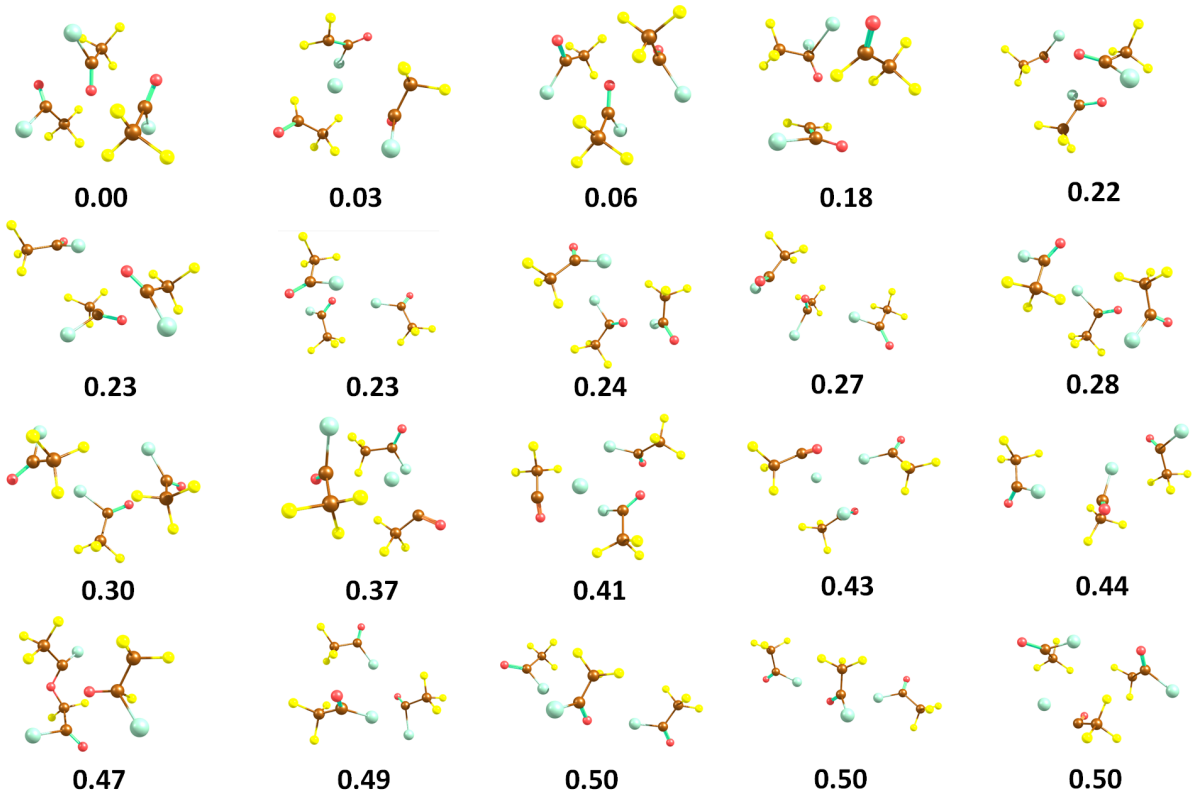

Fig. S19 Selected structures of anionic CF_3COCl trimer clusters obtained through genetic algorithm optimization as optimized at the B3LYP-D3/aug-cc-pVDZ level along with the relative energy (in eV).

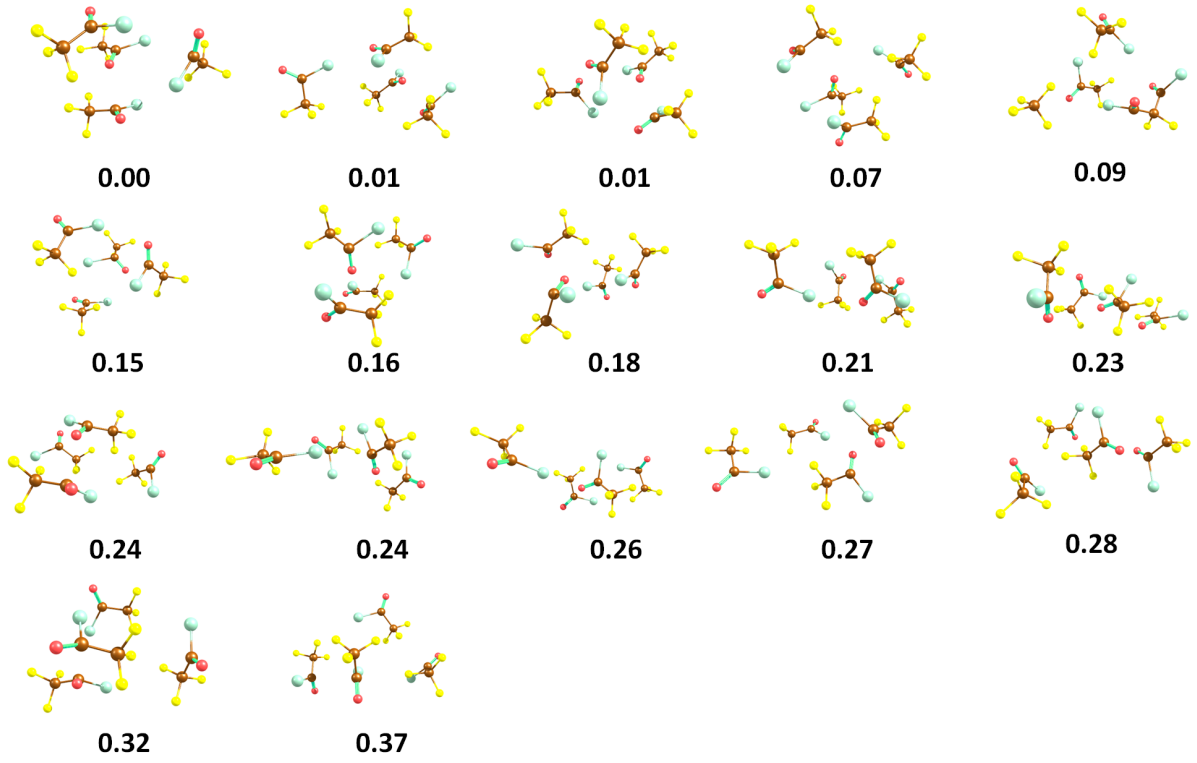

Fig. S20 Selected structures of anionic CF_3COCl tetramer clusters obtained through genetic algorithm optimization as optimized at the B3LYP-D3/aug-cc-pVDZ level along with the relative energy (in eV).

5 Cartesian coordinates of optimized molecules and ions (in Å) along with the relative energy (in Hartree) at the B3LYP-D3/aug-cc-pVTZ level

M
E = -911.353865
C 0.081147 0.799924 0.000000
C 0.542694 -0.689739 0.000000
F 0.081147 -1.317833 1.087907
F 1.870925 -0.751042 0.000000
F 0.081147 -1.317833 -1.087907
O 0.822665 1.714815 0.000000
Cl -1.683725 0.947103 0.000000

M_2
E = -1822.712194
6 -1.647009 0.428905 0.528661
6 -2.383901 -0.835357 -0.010297
9 -3.648963 -0.832087 0.436975
9 -1.777381 -1.932845 0.433046
9 -2.401405 -0.855239 -1.343318
8 -0.774178 0.387300 1.320505
17 -2.293561 1.922751 -0.154682
6 1.687641 -0.540829 -0.445209
6 2.231712 0.861641 -0.033643
9 2.375250 0.952945 1.288596
9 1.392204 1.808194 -0.446966
9 3.424654 1.062692 -0.612445
8 0.725257 -0.698193 -1.108462
17 2.692472 -1.854042 0.170187

M_2
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C -2.174226 -0.264092 -0.628313
C -1.772343 1.021218 0.157886
F -2.818923 1.460390 0.866718
F -1.393969 1.971935 -0.690008
F -0.760782 0.773884 1.003318
O -2.274023 -0.304700 -1.800760
Cl -2.492536 -1.629400 0.450750
C 2.174404 0.264024 0.628336
C 1.773838 -1.021634 -0.157958
F 0.759380 -0.775986 -1.000436
F 1.400085 -1.974076 0.690033
F 2.819581 -1.457545 -0.870009
O 2.275803 0.304233 1.800663
Cl 2.488264 1.630531 -0.450484

M_2
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C -2.644244 0.449301 0.378541
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F -2.564340 0.929908 1.615543
F -3.904453 0.061850 0.144037
O -1.071028 -1.235815 1.111228
Cl -1.644836 -1.373304 -1.442157
C 2.555426 0.851766 -0.329471
C 2.497707 -0.550657 0.349315
F 1.951647 -0.451433 1.564881
F 3.726780 -1.044548 0.466286
F 1.762947 -1.389352 -0.390537
O 3.551309 1.378408 -0.670093
Cl 0.939512 1.560739 -0.528099

M_2
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C -0.549703 -1.550135 -0.281623
C -2.097993 0.505944 -0.256795
Cl -2.086823 2.267710 -0.452996
Cl -0.572145 0.087946 1.923704
F -1.411448 -2.349727 0.338909
F 3.094256 1.725597 -0.209569
F -0.744364 -1.636046 -1.603953
F 0.285470 0.631057 -0.445833
F 0.692300 -1.957749 -0.008736
F 2.997375 -0.034776 0.987815
O -3.062167 -0.158417 -0.396302
O 3.336977 -0.249855 -1.197704

M_3
E = -2734.072738
C 2.237722 -0.241010 0.531856
C 2.856324 -0.302172 -0.898211
F 4.119923 0.147679 -0.836898
F 2.163114 0.478364 -1.721205
F 2.868968 -1.543950 -1.380655
O 1.432923 0.556127 0.860823
Cl 2.924376 -1.451630 1.615668
C -1.046225 -1.795968 -0.007939
C -2.486094 -1.822728 -0.605939
F -3.026345 -3.035296 -0.425648
F -2.437368 -1.564830 -1.910066
F -3.261662 -0.912940 -0.011764
O -0.075515 -1.628164 -0.657978
Cl -1.036725 -2.064418 1.733043
C -0.297116 2.596914 -0.444029
C -1.067873 2.494837 0.906910
F -2.207130 3.198890 0.800805
F -0.336809 3.008927 1.889113
F -1.382070 1.232852 1.214390
O 0.634391 3.295764 -0.611569
Cl -1.041792 1.606852 -1.712754

M_3
E = -2734.062234
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C -2.521441 -1.515798 -0.008079
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F -3.043536 -2.732954 0.104178
F -2.284210 -1.031485 1.216902
O -4.552366 -0.932359 -1.194728
Cl -2.884932 1.072507 -0.914740
C 0.640400 -2.207786 2.661178
C 3.342002 -0.967601 -0.396188
F 4.563546 -1.357902 -0.755560
F 3.144608 -1.308673 0.875207
F 3.279005 0.361066 -0.493124
O 0.236375 -2.840328 1.821972
Cl 2.122960 -1.724142 -1.437515
C 0.276516 1.530785 0.779217
C 0.550143 2.452928 -0.448385
F -0.481709 3.272891 -0.679640
F 0.757879 1.712436 -1.532410
F 1.639850 3.194038 -0.210237
O 0.445440 0.365146 0.766711
Cl -0.270750 2.439319 2.192624

M_3
E = -2734.070600
C -2.515576 -1.212859 -0.733892
C -2.112428 -1.472646 0.749980
F -1.747845 -0.337693 1.355872
F -1.096739 -2.330439 0.799331
F -3.150887 -1.997266 1.414838
O -2.020824 -1.764234 -1.649520
Cl -3.824661 -0.032595 -0.867720
C 2.754810 -1.254085 -0.626387
C 2.422362 -1.157484 0.894636
F 1.344921 -0.382540 1.096826
F 3.450660 -0.631548 1.552562
F 2.167917 -2.374514 1.387190
O 3.807244 -0.972328 -1.077481
Cl 1.384239 -1.840240 -1.565702
C 0.164176 1.862379 -0.647790
C -0.282350 2.828875 0.491242
F 0.458025 2.622241 1.585014
F -1.560639 2.615651 0.786385
F -0.134326 4.100736 0.102413
O -0.536004 1.043180 -1.124305
Cl 1.842242 2.132854 -1.136000

M_3
E = -2734.062047
C -0.054813 2.264011 1.144861
C -0.509501 2.590084 -0.300373
F -0.904228 1.497494 -0.954948
F 0.483855 3.164561 -0.973353

F -1.543757 3.446739 -0.239056
O 0.888566 2.702122 1.691268
Cl 2.326502 -2.796579 0.214754
C -3.074875 -1.933645 0.233371
C -3.785883 -0.675997 -0.354759
F -5.100756 -0.875202 -0.391000
F -3.352315 -0.434116 -1.597610
F -3.533457 0.396391 0.405741
O -3.650823 -2.892980 0.604314
Cl -1.319417 -1.741759 0.276556
C 2.582793 -0.064415 -0.090694
C 3.377388 -1.412880 -0.132790
F 3.924414 -1.554797 -1.350955
F -0.936922 1.442358 1.722117
F 4.370428 -1.360794 0.768692
O 1.428094 0.032202 0.135848
Cl 3.628050 1.312609 -0.429886

M^+
E = -910.939046
C 0.012642 1.047676 0.000000
C 0.554184 -0.975075 0.000000
F 0.012642 -1.395152 1.086804
F 1.829737 -0.914204 0.000000
F 0.012642 -1.395152 -1.086804
O 0.967894 1.693347 0.000000
Cl -1.637606 1.138718 0.000000

M_2^+
E = -1822.320722
C 1.949314 -0.213110 -0.000787
C 3.429180 0.411678 0.000018
F 4.044230 -0.019656 1.088791
F 3.349142 1.725085 0.000129
F 4.045261 -0.019370 -1.088272
O 1.010687 0.537972 -0.000781
Cl 1.879139 -1.906531 0.000410
C -1.949315 0.213115 -0.000272
C -3.429176 -0.411683 0.000100
F -4.044461 0.019488 1.088800
F -3.349127 -1.725090 0.000057
F -4.045028 0.019519 -1.088264
O -1.010680 -0.537958 -0.000458
Cl -1.879152 1.906538 -0.000152

M_2^+
E = -1822.355184
C 0.812556 1.969140 0.000428
C -1.704803 -0.738922 -0.708234
C 3.019789 -0.948145 -0.000110
C -1.704741 -0.739479 0.707787
Cl -2.830687 0.019277 -1.651607
Cl -2.830514 0.018021 1.651856
F -0.753257 -1.382607 -1.288710
F 4.069527 -0.169794 -0.000071
F 1.502429 2.267189 1.065270
F -0.753162 -1.383645 1.287677
F 1.502325 2.267607 -1.064367
F 3.408459 -2.195432 -0.000482
O 1.896249 -0.582210 -0.000055
O -0.281659 1.517274 0.000392

M_2^+
E = -1822.301585
C -1.084760 -0.692044 0.084577
C -2.264725 0.201654 0.592466
F -2.820643 0.840634 -0.433342
F -1.798546 1.085644 1.466319
F -3.171857 -0.575212 1.182633
O 0.019566 -0.600501 0.532534
Cl -1.532621 -1.811939 -1.159068
C 2.328803 -1.401862 -0.055212
C 1.220861 2.211490 -0.852450
F 0.014386 1.926370 -1.290259
F 1.218889 2.575066 0.408875
F 2.047191 1.165940 -1.037770
O 2.107080 -1.852783 -1.059390
Cl 2.849150 -0.861893 1.331447

M_3^+
E = -2733.687265
C -2.547352 0.081811 0.336918
C -3.777504 -0.512746 -0.495044
F -3.641366 -1.830434 -0.525195
F -3.762353 -0.019212 -1.715646
F -4.894581 -0.175245 0.129696
O -1.797440 0.843408 -0.209258
Cl -2.439984 -0.451590 1.945524
C 0.827860 2.059620 0.567066
C 0.876688 2.181383 -1.013966
F -0.009880 3.121203 -1.335017
F 0.536107 1.028854 -1.566142
F 2.080917 2.536360 -1.410506
O -0.082216 1.529910 1.152109
Cl 2.058620 2.835431 1.451353
C 2.565345 -1.284228 0.035802
C 1.296220 -2.188439 -0.060281
F 1.186169 -2.704999 -1.281455
F 0.202579 -1.439689 0.183768
F 1.341742 -3.167127 0.838170
O 2.499640 -0.114977 0.238945
Cl 4.042457 -2.162579 -0.193135

M_3^+
E = -2733.655127
6 2.049739 3.855437 -0.210504
6 -0.479767 1.533538 -0.848795
9 0.610150 1.420944 -1.540725
9 -1.256478 2.479736 -1.304605
9 -3.203025 0.897371 -0.361251
8 2.907048 4.533227 -0.451045
17 0.074748 2.154427 0.924944
6 -2.205144 0.120921 0.026545
6 -2.595581 -1.396645 -0.120370
9 -1.593778 -2.163049 0.284916
9 -2.857345 -1.624569 -1.399753
9 -3.674707 -1.624023 0.615410
8 -1.052327 0.320710 -0.713471
17 -1.866594 0.481830 1.806995
6 2.530983 -2.306389 -0.234046
6 2.364442 -1.124529 0.767158
9 2.653404 0.046956 0.170958
9 3.152239 -1.280658 1.812889
9 1.084231 -1.054000 1.194330
8 3.257424 -3.210992 -0.054432
17 1.490822 -2.114252 -1.660047

M_3^+
E = -2733.697209
C -0.404245 -0.805958 -0.346652
C 0.760862 2.345360 -0.051749
C -4.254227 -1.108540 -0.116791
C -0.633982 1.621653 0.029020
C 3.235810 -1.275452 0.324128
C -0.334527 -2.081995 0.237093
Cl 1.762946 1.630412 -1.338762
Cl -1.641479 2.274292 1.297464
Cl 4.864246 -1.529257 -0.135201
F -0.488845 -0.737787 -1.626970
F -1.249071 1.658935 -1.142895
F -5.020195 -0.075728 -0.333407
F 3.147968 -0.450189 1.356639
F 0.535320 3.628468 -0.310474
F -0.271991 -2.238379 1.501889
F -0.339511 -3.137753 -0.476842
F 1.377002 2.224871 1.123585
F -4.990274 -2.167214 0.068992
O 2.275832 -1.750446 -0.188061
O -0.364594 0.222751 0.417486
O -3.071102 -1.084809 -0.091235

M^-
E = -911.401536
C -0.270959 0.805485 -0.417539
C 0.842060 -0.179080 -0.024567
F 0.955785 -0.434386 1.307614
F 2.041568 0.358932 -0.399129
F 0.758880 -1.371538 -0.641979
O -0.263440 1.932159 0.030538
Cl -2.066187 -0.364281 0.000575

M_2^-
E = -1822.778113
C 1.274502 0.350256 -0.208572
C 2.437223 -0.579793 -0.022653
F 3.353000 -0.529505 -1.052043
F 2.015122 -1.857484 0.029231
F 3.153687 -0.342159 1.099600

O 0.289393 0.072624 -0.890937
Cl 1.777786 2.103426 0.059650
C -1.428778 -0.438567 0.556567
C -2.316139 0.633965 -0.082673
F -2.475452 0.510564 -1.403434
F -1.843483 1.856517 0.178285
F -3.570941 0.574266 0.466281
O -0.876347 -0.301313 1.607035
Cl -1.824411 -2.096098 -0.121185

M_2^-
E = -1822.780193
C 2.107884 0.603576 0.506667
C 2.170281 -0.791436 -0.173986
F 1.207187 -1.046017 -1.050298
F 2.219295 -1.766561 0.730262
F 3.351839 -0.824632 -0.861183
O 2.708340 0.853889 1.494320
Cl 1.611653 1.888019 -0.674536
C -3.363202 0.024364 0.101909
C -2.147671 -0.354132 -0.531582
F -1.905281 -1.632517 -0.738119
F -3.562378 1.378543 0.008482
F -1.558555 0.419477 -1.422444
O -4.135983 -0.673631 0.701831
Cl -0.373509 0.047809 1.439974

M_2^-
E = -1822.769522
C 2.201714 -0.353111 0.531644
C 1.666705 1.060143 0.167028
F 2.717575 1.914341 0.359379
F 0.699479 1.430385 0.995435
F 1.269471 1.208400 -1.087890
O 2.273225 -0.745833 1.640786
Cl 3.136656 -1.087725 -0.825590
C -2.127810 -0.550777 0.878453
C -2.741693 0.312902 -0.250049
F -1.875754 1.176603 -0.793590
F -3.741648 1.060501 0.301089
F -3.304246 -0.391252 -1.257411
O -2.788991 -1.371256 1.445866
Cl -0.298495 -1.469277 -0.310220

M_2^-
E = -1822.745907
C -1.132444 0.103910 0.280461
C -2.329608 -0.536275 -0.534598
C 1.222194 0.331405 -0.065096
C 2.234061 -0.767620 0.125582
Cl -1.450341 1.865104 0.618998
Cl 1.877451 1.852718 -0.595369
F -0.890766 -0.477189 1.478750
F -1.956582 -1.956581 -0.491457
F -3.402104 -0.525518 0.453012
F 3.278009 -0.350026 0.874702
F 2.758476 -1.209591 -1.049155
F 1.684137 -1.823180 0.733226
O -2.586415 -0.074978 -1.633881
O 0.028087 -0.039115 -0.520057

M_3^-
E = -2734.149492
C -2.214428 -0.755933 0.540397
C -2.071908 -1.464313 -0.821193
F -0.976386 -2.206743 -0.946034
F -2.118561 -0.580101 -1.817683
F -3.142001 -2.300731 -0.976437
O -2.844589 0.239320 0.694664
Cl -1.702281 -1.814563 1.906254
C 2.297456 -0.106891 -0.527075
C 2.436356 -1.145493 0.599415
F 1.555254 -2.141883 0.542675
F 2.354427 -0.558604 1.793926
F 3.679613 -1.709596 0.515624
O 2.641673 1.027585 -0.423065
Cl 1.958224 -0.884138 -2.118631
C -0.112980 1.489090 0.412368
C -0.426737 2.569269 -0.585924
F -1.657340 3.131295 -0.405053
F -0.403831 2.075392 -1.834797
F 0.446440 3.608723 -0.542961
O -0.032947 0.287316 0.156669
Cl 0.026516 2.121764 2.089000

M_3^-
E = -2734.147081
C -2.188511 -0.635869 -0.811706
C -2.435064 -1.352928 0.532600
F -2.377780 -0.565851 1.603450
F -1.586920 -2.366166 0.685617
F -3.695650 -1.882798 0.495505
O -1.856458 -1.206735 -1.798669
Cl -2.896632 1.021793 -0.831646
C 1.844417 -1.374656 0.738607
C 1.955816 -1.715593 -0.764859
F 2.167006 -0.669348 -1.558796
F 0.878488 -2.373645 -1.179430
F 3.026539 -2.552327 -0.915240
O 1.323932 -2.091613 1.526637
Cl 2.963068 -0.044607 1.210747
C 0.079098 1.391780 0.326205
C 0.577222 2.399904 -0.663552
F -0.143487 3.553338 -0.662839
F 0.533876 1.900310 -1.910311
F 1.872515 2.797054 -0.449723
O -0.015524 0.176532 0.115067
Cl -0.106714 2.089497 1.981950

M_3^-
E = -2734.150309
C -1.069225 2.726598 -0.537468
C -1.161576 2.440354 0.849925
F -2.274443 2.068018 1.439397
F -0.344473 3.057497 1.677165
F -3.016549 -0.911956 0.644911
O -0.173139 3.313903 -1.086015
Cl -2.462603 2.030781 -1.484686
C 2.382826 -0.765872 -0.548692
C 3.004028 0.611374 -0.176957
F 3.117374 0.840508 1.125176
F 2.340499 1.601598 -0.752437
F 4.267410 0.601090 -0.695706
O 1.874815 -0.979418 -1.589706
Cl 2.870114 -2.061997 0.590424
C -2.123483 -1.896986 0.821663
C -1.548072 -2.349204 -0.542281
F -1.443762 -1.385266 -1.443892
F -2.432807 -3.269852 -1.035333
F -0.379968 -2.962988 -0.393938
O -2.012537 -2.500777 1.828891
Cl 0.008982 0.030329 1.040698

M_3^-
E = -2734.136906
C 2.301954 -1.100706 -0.474585
C 3.205994 0.080532 -0.019285
F 3.244285 0.284803 1.289886
F 2.867118 1.202084 -0.640109
F 4.471915 -0.243454 -0.415785
O 1.852474 -1.180921 -1.561229
Cl 2.360178 -2.477661 0.670169
C -0.916445 2.455827 0.988150
C -0.688631 2.859441 -0.492271
F -1.189884 1.980592 -1.362836
F 0.601571 3.075324 -0.812839
F -1.346799 4.036206 -0.696436
O -0.496530 3.121708 1.881794
Cl 0.049299 0.221484 0.928765
C -2.437620 -1.461921 0.707774
C -1.909200 -1.944028 -0.674434
F -2.892471 -2.734141 -1.196668
F -0.827586 -2.700513 -0.524933
F -1.667554 -0.981019 -1.548245
O -2.314176 -2.097068 1.693819
Cl -3.528055 -0.059326 0.568390

CF_3CO^+
E = -450.732299
C -1.182348 0.000055 0.000000
C 0.505471 -0.000131 0.000000
F 0.828835 -0.626080 1.084220
F 0.828835 1.251874 0.000000
F 0.828835 -0.626080 -1.084220
O -2.289660 0.000379 0.000000

CF_3^+
E = -337.352728

C 0.000000 0.000013 0.000000
F 1.180643 0.367705 -0.000000
F -0.271871 -1.206315 -0.000000
F -0.908773 0.838601 0.000000

$COCl^+$
E = -573.230097
C 0.000000 0.000000 -0.572388
O 0.000000 0.000000 -1.693697
Cl 0.000000 0.000000 0.999053

CF_2Cl^+
E = -697.723903
C 0.000000 0.000000 -0.381698
F 0.000000 1.061693 -1.046741
F -0.000000 -1.061693 -1.046741
Cl -0.000000 -0.000000 1.243031

CF_2^+
E = -237.373601
C -0.000000 0.000000 0.424211
F 0.000000 1.081157 -0.141404
F -0.000000 -1.081157 -0.141404

$M.COCl^+$
E = -1484.603787
C 1.061424 0.944543 -0.065648
C 0.925370 -0.610062 0.023037
Cl 2.423605 -1.445729 -0.029913
O -0.142962 -1.141612 0.118166
F 1.740146 1.413215 0.970816
F -0.181849 1.481989 -0.043848
F 1.649807 1.298408 -1.199075
O -2.217419 -0.040629 1.712819
C -2.388740 -0.163293 0.610166
Cl -2.869382 -0.278489 -0.887984

$M_2.COCl^+$
E = -2395.965467
C -2.625566 -1.016086 0.699431
C -2.741830 0.248067 -0.212274
O -1.900036 1.095538 -0.237950
Cl -4.173916 0.280361 -1.174601
Cl 1.005259 -0.731980 -1.194847
C 2.748925 -1.124168 -0.932644
C 3.306436 -0.393724 0.325097
O 3.361514 -1.841924 -1.621943
F -1.523340 -0.907719 1.452200
F -2.522689 -2.105149 -0.060209
F -3.684299 -1.118467 1.493553
F 3.072677 0.943045 0.214229
F 2.675399 -0.821540 1.420994
F 4.599338 -0.588042 0.441306
C 0.402438 1.835079 0.787946
O 0.375177 1.203528 1.714301
Cl 0.533985 2.829777 -0.424626

$M.CF_3CO^+$
E = -1362.115819
C 1.504305 -0.939659 -0.137774
C 1.198970 0.565071 0.178786
Cl 2.496965 1.621460 -0.008428
O 0.098132 0.960625 0.528210
F 1.847770 -1.053399 -1.409612
F 0.393143 -1.660759 0.086655
F 2.471394 -1.371930 0.650565
O -1.465113 -0.420925 2.028697
C -1.453079 -0.051338 0.965620
C -2.290553 0.177672 -0.353721
F -1.557502 -0.147713 -1.394569
F -3.346564 -0.594168 -0.248310
F -2.616064 1.450980 -0.376889

$M_2.CF_3CO^+$
E = -2273.484785
C -1.915449 -1.593989 0.699672
C -2.432553 -0.397130 -0.163220
O -1.907491 0.682438 -0.159061
Cl -3.816413 -0.763286 -1.104792
Cl 1.061912 -0.981609 -1.525423
C 1.928276 -0.302803 -0.191951
C 3.325445 -0.966120 0.063137
O 1.525783 0.591355 0.495467
F -0.795594 -1.219289 1.335743
F -1.639986 -2.635222 -0.077482
F -2.833087 -1.926309 1.598128
F 3.143267 -2.255567 0.342620
F 4.073585 -0.843875 -1.030307
F 3.917682 -0.365502 1.082638
F -1.215198 3.518235 -0.175479
C -0.123086 2.789249 -0.170222
C -0.311251 1.770868 1.033937
F 0.054553 2.167670 -1.299205
F 0.931839 3.499902 0.165698
O -0.460209 1.526504 2.114135

$M.CF_3^+$
E = -1248.752155
C -1.102118 -0.921155 -0.004357
C -0.644853 0.593362 -0.023548
O 0.547753 0.974845 -0.012837
Cl -1.823744 1.756243 -0.008700
F -0.292321 -1.623490 -0.783910
F -2.341040 -1.019795 -0.430551
F -1.007456 -1.325836 1.256372
F 1.731555 -0.822872 0.860649
C 1.877915 0.132564 -0.002621
F 2.736572 1.018838 0.361202
F 2.043352 -0.280569 -1.215567

$M_2.CF_3^+$
E = -2160.123582
C 1.502069 -1.153751 -0.947072
C 1.436062 -0.682151 0.555051
O 1.835736 0.428736 0.985540
Cl 1.059734 -1.835897 1.691265
Cl -2.534795 -1.734148 0.139140
C -1.969870 -0.097516 0.057237
C -3.113727 0.962031 -0.084830
O -0.818523 0.218054 0.106646
F 1.266967 -0.149207 -1.771904
F 0.636095 -2.123833 -1.153859
F 2.745771 -1.603528 -1.113609
F -3.809205 0.715489 -1.192245
F -3.915413 0.885895 0.975986
F -2.581121 2.175363 -0.153619
F 3.267787 1.237957 -0.617325
C 2.342757 1.650569 0.201144
F 2.813456 2.397861 1.144872
F 1.326172 2.179707 -0.400915

$M.CF_2COCl^+$
E = -1722.467758
C 1.746955 -0.826388 0.055419
C 0.814847 0.435391 -0.045520
Cl 1.604237 1.852869 -0.613190
O 0.083609 0.626193 1.103188
F 2.326910 -1.059606 -1.109287
F 0.977925 -1.869819 0.391383
F 2.647090 -0.609504 0.995224
O -0.255078 0.021938 -1.103648
C -1.363666 -0.069695 -0.530015
Cl -2.749359 -0.496056 -1.293073
C -1.253161 0.277555 0.980908
F -1.562569 -0.772714 1.723461
F -2.037247 1.294748 1.293153

$M_2.CF_2COCl^+$
E = -2633.829248
C -1.426945 1.535694 0.799990
O -1.936438 0.304721 1.184904
C -1.708394 -0.692056 0.262389
O -0.745090 -0.045072 -0.759509
C -0.581270 1.158010 -0.448570
C -2.992378 -1.022449 -0.582434
F -3.915877 -1.507873 0.225887
Cl -0.943071 -2.082834 0.928708
Cl 0.342829 2.200045 -1.307610
F -2.382878 2.385370 0.443879
F -0.703539 2.067174 1.765567
F -2.698983 -1.889699 -1.536993
F -3.422952 0.119566 -1.132303
C 3.237208 -0.640265 0.771505
C 3.223207 -0.411303 -0.768773
F 4.151644 -1.138018 -1.350975
F 2.013358 -0.760073 -1.258482
F 3.420127 0.883790 -1.045754

Cl 1.956073 0.336519 1.592963
O 3.968304 -1.349816 1.344465

$M.C_2FCl_2^+$
E = -2007.532984
C 1.558854 -0.794294 0.667874
F 1.747058 -1.859325 -0.094398
C 1.332957 0.451942 -0.268124
O 0.241038 1.052351 -0.463062
C -1.087735 0.692048 -0.056167
C -1.588226 -0.469740 -0.497872
F -0.791296 -1.297115 -1.161615
F 0.515095 -0.969487 1.464856
F 2.636140 -0.553306 1.396987
Cl 2.670594 1.057865 -1.037353
Cl -1.859518 1.949004 0.753833
Cl -3.174980 -0.982484 -0.294259

Cl
E = -460.175331
cl 0.000000 0.000000 0.000000

COCl
E = -573.545430
O 1.056453 1.309882 0.000000
C 0.000000 0.845150 0.000000
Cl -0.497154 -0.914704 0.000000

CF_3
E = -337.692177
C -0.274952 0.173217 0.000000
F -0.274952 -0.571888 1.091901
F 0.733205 1.028297 0.000000
F -0.274952 -0.571888 -1.091901

OCF
E = -213.181133
O 1.141740 0.182473 0.000000
C 0.000000 0.421148 0.000000
F -1.014880 -0.442963 0.000000

COClF
E = -673.482361
C -0.000000 0.511357 0.000000
F 1.316367 0.711825 0.000000
O -0.796787 1.371581 0.000000
Cl -0.321942 -1.202777 0.000000

CF_2COCl
E = -811.417175
C -0.000000 0.647555 -0.000000
C -0.780859 -0.542741 0.000000
F -0.311467 -1.758247 0.000000
F -2.083089 -0.493659 0.000000
O -0.466076 1.756101 0.000000
Cl 1.762633 0.328792 -0.000000

F
E = -99.766141
F 0.000000 0.000000 0.000000

CF_4
E = -437.653605
C 0.000000 0.000000 0.000000
F 0.766252 0.766252 0.766252
F -0.766252 -0.766252 0.766252
F -0.766252 0.766252 -0.766252
F 0.766252 -0.766252 -0.766252

CF_3CO
E = -451.056279
C 0.527028 -1.142278 0.000000
C 0.044806 0.352060 0.000000
F 0.527028 0.955840 1.089225
F -1.286441 0.465135 0.000000
F 0.527028 0.955840 -1.089225
O -0.167442 -2.081252 0.000000

CO
E = -113.353803
C 0.000000 0.000000 -0.643332
O 0.000000 0.000000 0.482499

Cl^-
E = -460.310516
Cl 0.000000 0.000000 0.000000

CF_3^-
E = -337.759296
C -0.376723 0.398135 -0.000000
F -0.376723 -0.524437 1.098214
F 1.004596 0.783450 -0.000000
F -0.376723 -0.524437 -1.098214

CF_3Cl^-
E = -798.024349
Cl -2.017452 -0.023139 -0.000000
C 0.622073 0.011455 0.000000
F 1.132009 -0.616654 1.088907
F 1.132009 1.269379 0.000000
F 1.132009 -0.616654 -1.088907

$COCl^-$
E = -573.670702
C 0.592685 -1.515226 0.000000
O -0.444513 -1.973014 0.000000
Cl -0.000000 1.463263 0.000000

F^-
E = -99.895852
F 0.000000 0.000000 0.000000

$M.Cl^-$
E = -1371.696495
C -0.298472 1.034680 -0.000000
F -0.046636 1.803463 1.082765
C 0.656485 -0.193802 0.000000
O 1.841336 -0.023642 0.000000
F -1.605965 0.760136 -0.000000
F -0.046636 1.803463 -1.082765
Cl -0.046636 -1.298814 1.588944
Cl -0.046636 -1.298814 -1.588944

$M_2.Cl^-$
E = -2283.059057
C 1.736602 -0.991473 0.101435
C 2.907871 -0.039688 0.471872
O 3.463852 -0.140576 1.521346
Cl 3.988040 0.151389 -1.108328
Cl -1.453247 1.309095 0.018679
C -3.133542 0.907363 -0.174338
C -3.405075 -0.623045 -0.028771
O -4.012984 1.676261 -0.392012
F 1.103853 -0.719283 -1.040841
F 0.827244 -1.025359 1.088095
F 2.234630 -2.250737 -0.011903
F -2.721325 -1.319605 -0.944941
F -3.051399 -1.053971 1.189784
F -4.709128 -0.880346 -0.197814
Cl 1.735974 1.918297 0.383926

$M.CF_3^-$
E = -1249.159503
C -1.544290 -0.600375 -0.040951
C -0.399436 0.277512 -0.435033
Cl -0.910371 2.016797 0.015476
O 0.645096 -0.078948 0.531938
F -1.233304 -1.909002 -0.276286
F -2.658123 -0.327423 -0.764218
F -1.969048 -0.592881 1.278225
C 1.862924 -0.156374 0.019365
F 2.729027 -0.436650 1.028997
F 2.026098 -1.137196 -0.902574
F 2.305388 0.983314 -0.561799

$M_2.CF_3^-$
E = -2160.525239
C -1.911985 -1.783341 0.123187
C -1.227102 -0.461098 0.017257
O -2.249654 0.441094 -0.482211
Cl 0.029545 -0.617705 -1.324961
Cl 2.348095 2.055529 -0.411139
C 2.021618 0.573114 0.556187
C 2.989085 -0.578229 0.185402
O 1.302236 0.546309 1.487905
F -2.880726 -1.732217 1.079223

F -1.052511 -2.766447 0.479411
F -2.568782 -2.272329 -0.995171
F 3.229899 -0.696663 -1.121288
F 4.182758 -0.322806 0.789458
F 2.542806 -1.739017 0.653201
F -3.226228 2.380104 -0.499678
C -2.251938 1.643150 0.089333
F -1.098653 2.329947 -0.059857
F -2.523966 1.630115 1.412473

$M.Cl_2^-$

E = -1831.891664
C -1.547190 -0.000381 -0.469793
F -1.823340 1.081785 -1.223189
C -0.033447 0.000013 -0.064911
O 0.731584 -0.000404 -1.038005
F -2.403471 0.000166 0.561028
F -1.823118 -1.083539 -1.221852
Cl 0.139457 1.528023 1.133379
Cl 0.139855 -1.526537 1.135053
Cl 3.137188 -0.000326 -0.593821

CO_2

E = -188.651912
O 0.000000 0.000000 1.160570
C 0.000000 0.000000 0.000000
O 0.000000 0.000000 -1.160570

6 Cartesian coordinates of optimized molecules and ions (in Å) along with the relative energy (in Hartree) for the genetic algorithm runs at the B3LYP-D3/aug-cc-pVDZ level

M_2

E = -1822.441167
C 1.643097 0.456184 -0.511185
C 2.312295 -0.856165 -0.001820
F 3.566876 -0.932618 -0.494050
F 1.618575 -1.916337 -0.431783
F 2.373808 -0.886236 1.337131
O 0.739284 0.476758 -1.278677
Cl 2.407899 1.908015 0.157308
C -1.663001 -0.509871 0.470945
C -2.241850 0.867797 0.027387
F -2.355855 0.941007 -1.306581
F -1.443421 1.854068 0.452872
F -3.463242 1.034690 0.576018
O -0.718915 -0.627760 1.178922
Cl -2.592421 -1.872181 -0.175918

E = -1822.441051
C 1.596115 0.506129 0.546274
C 2.417894 -0.691931 -0.017896
C -1.840592 0.506534 -0.466512
C -1.960408 -0.989742 -0.047145
Cl 2.141420 2.060904 -0.099978
Cl -3.133737 1.505118 0.220919
F 2.290464 -0.757769 -1.354388
F 1.980806 -1.837046 0.516957
F 3.722165 -0.543343 0.285689
F -2.040158 -1.120733 1.284468
F -0.895157 -1.670564 -0.489737
F -3.070410 -1.519142 -0.601669
O 0.705888 0.383581 1.320813
O -0.993143 0.920050 -1.185338

E = -1822.440793
C -1.571780 -0.102886 -0.059575
C -3.012660 0.463886 -0.235952
F -3.759672 -0.386114 -0.964960
F -2.965519 1.643966 -0.863206
F -3.596379 0.632806 0.964705
O -0.598984 0.458574 -0.444534
Cl -1.555346 -1.662801 0.770536
C 2.066726 0.265075 0.719181
C 2.429730 -0.632486 -0.501637
F 2.074003 -0.077754 -1.668419
F 1.828293 -1.823419 -0.386681
F 3.767672 -0.824605 -0.508681
O 1.590400 -0.153613 1.719733
Cl 2.523640 1.963675 0.471316

E = -1822.440598
C 1.543735 0.062387 0.023369
C 3.015089 -0.422602 0.192549
F 3.567776 -0.655961 -1.012280
F 3.044292 -1.551228 0.907826
F 3.741991 0.514959 0.828176
O 0.609912 -0.511459 0.477765
Cl 1.429945 1.556998 -0.918477
C -2.241538 -0.037400 0.857093
C -2.407259 -0.718792 -0.534034
F -3.686360 -0.556903 -0.939032
F -2.150981 -2.027506 -0.435522
F -1.599552 -0.187841 -1.466130
O -2.218660 -0.633323 1.878792
Cl -2.185514 1.739298 0.740025

E = -1822.440411
C 1.890088 0.823112 0.395111
C 2.615148 -0.253602 -0.466401
F 3.679701 -0.719762 0.221363
F 3.046764 0.293629 -1.607371
F 1.807090 -1.284264 -0.754130
O 1.900587 1.981067 0.155854
Cl 1.084532 0.112220 1.822364
C -1.670122 0.439466 -0.561346
C -2.122985 -0.951048 -0.021350
F -2.316655 -0.899453 1.309002
F -1.189880 -1.870285 -0.287567
F -3.276308 -1.318632 -0.611722
O -0.653579 0.619217 -1.145055
Cl -2.849546 1.713608 -0.209932

E = -1822.440375
C 0.711420 0.064665 0.146100
C -3.144679 -0.424737 -0.261461
C 0.539525 1.560250 -0.261175
C 2.104770 -0.488260 -0.254642
Cl 2.118685 -2.257494 -0.445326
Cl 0.526183 -0.127393 1.914542
F 1.390399 2.358065 0.393021
F -3.040171 -1.746131 -0.185174
F 0.753658 1.678006 -1.585355
F -0.277574 -0.626281 -0.494561
F -0.716402 1.956437 0.002738
F -3.018498 0.059069 0.969072
O 3.066707 0.190940 -0.395080
O -3.323166 0.203946 -1.240830

E = -1822.440146
C -2.168383 0.258543 0.629994
C -1.765355 -1.024506 -0.156864
F -2.817638 -1.467135 -0.869997
F -1.382850 -1.982672 0.692510
F -0.749218 -0.774419 -1.008850
O -2.265083 0.300115 1.809234
Cl -2.498837 1.629452 -0.449759
C 2.168919 -0.258038 -0.630286
C 1.766617 1.024794 0.157334
F 0.746695 0.775508 1.005192
F 1.389346 1.985281 -0.691758
F 2.817196 1.463723 0.874997
O 2.267370 -0.298623 -1.809408
Cl 2.495256 -1.630585 0.448669

E = -1822.439786
C -1.733018 0.797372 0.247099
C -2.312779 -0.637523 0.430694
F -3.658350 -0.596927 0.368286
F -1.952450 -1.126912 1.621708
F -1.862848 -1.461706 -0.532345
O -1.114619 1.369164 1.079726
Cl -2.127218 1.480415 -1.345123
C 2.904821 0.094549 0.029493

C 1.714331 -0.832491 -0.359193
F 1.001224 -1.161764 0.735563
F 2.167096 -1.950626 -0.931877
F 0.894245 -0.202987 -1.226679
O 4.041199 -0.189966 -0.148945
Cl 2.353511 1.610366 0.765905

E = -1822.439735
C 1.788240 0.350107 0.670162
C 2.225678 -0.782877 -0.306208
F 1.618707 -0.640706 -1.498138
F 1.899318 -1.976726 0.204049
F 3.558689 -0.744203 -0.493378
O 1.252224 0.153660 1.707738
Cl 2.198381 1.962909 0.049097
C -2.667942 -0.597221 -0.130724
C -2.070244 0.841601 -0.115252
F -1.768326 1.206931 1.143074
F -2.950455 1.710655 -0.620630
F -0.943338 0.888100 -0.857439
O -3.768019 -0.848267 -0.491100
Cl -1.507757 -1.804631 0.460385

E = -1822.439412
C -1.673086 -0.772621 0.215889
C -2.610250 0.460138 0.391086
F -2.311964 1.428449 -0.495450
F -2.484946 0.956389 1.626475
F -3.890101 0.084707 0.200521
O -1.057383 -1.259397 1.102374
Cl -1.669464 -1.380880 -1.453514
C 2.549672 0.844811 -0.331127
C 2.475348 -0.553673 0.351669
F 1.908180 -0.446673 1.565673
F 3.706219 -1.057839 0.490731
F 1.742927 -1.397059 -0.399365
O 3.557831 1.369263 -0.661832
Cl 0.934962 1.565431 -0.557469

E = -1822.439136
C -2.932638 -0.423141 -0.563857
C -1.603095 -0.062299 0.163468
F -1.409129 1.268664 0.150004
F -0.571170 -0.650285 -0.463406
F -1.632569 -0.487146 1.436656
O -2.991569 -1.111984 -1.525573
Cl -4.342848 0.321499 0.219556
C 2.054012 0.585376 0.484783
C 2.682986 -0.768515 0.037687
F 2.259390 -1.119072 -1.188107
F 2.349464 -1.732706 0.902774
F 4.026205 -0.653336 0.013194
O 1.480036 0.737630 1.509483
Cl 2.324317 1.876810 -0.705662

E = -1822.438653
C 2.730668 0.733988 -0.129504
C 2.405930 -0.695613 0.399027
F 1.374470 -0.651152 1.262161
F 3.471589 -1.204153 1.026450
F 2.078142 -1.509011 -0.624274
O 3.774548 1.271320 0.027846
Cl 1.354804 1.457590 -0.988831
C -2.729648 -0.734465 -0.130931
C -2.407473 0.695119 0.399214
F -1.376678 0.651500 1.263173
F -3.474431 1.201515 1.026167
F -2.080044 1.509882 -0.623126
O -3.773099 -1.273218 0.024429
Cl -1.351621 -1.455602 -0.988816

E = -1822.435070
C -1.548518 1.172884 -0.151235
C -2.340964 -0.025372 0.414098
F -1.555277 -0.731105 1.240083
F -2.386765 2.077723 -0.683801
F -3.413783 0.407964 1.108588
O -0.371910 1.296242 -0.147082
Cl -2.877286 -1.061369 -0.944780
C 1.798870 -0.527800 0.631804
C 2.687271 0.486269 -0.149280
F 3.926861 -0.042872 -0.266242
F 2.774943 1.634065 0.530986
F 2.219336 0.741228 -1.378838
O 1.546754 -0.426130 1.783319
Cl 1.285136 -1.902149 -0.379880

E = -1822.426613
C 2.113243 -0.338101 0.729725
C 1.388836 0.848657 0.021045
C -0.024502 0.480169 -0.530594
C -2.081414 -0.203053 0.567586
Cl 2.792614 -1.528149 -0.402671
Cl -2.882661 -0.806619 -0.913727
F 1.233071 1.842057 0.924096
F -2.349119 -1.031373 1.584609
F 0.102797 -0.333118 -1.603791
F -0.644305 1.604942 -0.943165
F 2.137391 1.312724 -1.009995
F -2.579199 1.009831 0.869807
O -0.694489 -0.156503 0.499798
O 2.200502 -0.428567 1.907469

M_3

E = -2733.666758
C 2.237090 -0.240945 0.515978
C 2.815669 -0.316910 -0.928975
F 4.077647 0.164092 -0.911604
F 2.080568 0.436117 -1.753241
F 2.844586 -1.574484 -1.391370
O 1.420753 0.548982 0.856321
Cl 2.982361 -1.418138 1.609392
C -1.045766 -1.783696 -0.006771
C -2.493152 -1.807856 -0.583517
F -3.030054 -3.031575 -0.409611
F -2.466938 -1.532269 -1.892516
F -3.268360 -0.903905 0.037097
O -0.079572 -1.601502 -0.671039
Cl -1.006222 -2.078011 1.737041
C -0.294877 2.579909 -0.446322
C -1.028593 2.480472 0.924262
F -2.155482 3.223724 0.860018
F -0.252755 2.961604 1.898774
F -1.376027 1.217459 1.226570
O 0.655542 3.259164 -0.633658
Cl -1.105237 1.627568 -1.713372

E = -2733.666484
C 2.219044 0.372545 -0.130190
C 3.173971 -0.639753 0.570789
F 3.049709 -1.877383 0.069262
F 2.921635 -0.673002 1.882715
F 4.447571 -0.228173 0.384532
O 1.559099 1.160999 0.460847
Cl 2.284052 0.261185 -1.895793
C -0.982670 -1.917183 0.371511
C -1.700275 -2.013757 -1.008562
F -2.046137 -3.292879 -1.252240
F -0.879043 -1.598449 -1.978914
F -2.810200 -1.256982 -1.019811
O 0.140187 -1.561882 0.505699
Cl -2.027090 -2.419991 1.710658
C -0.898248 2.623359 0.875452
C -1.150719 2.420488 -0.647875
F -0.967391 1.145907 -1.033999
F -0.337520 3.206847 -1.358181
F -2.430056 2.762111 -0.916637
O -0.339255 3.562509 1.326680
Cl -1.632490 1.331796 1.860246

E = -2733.664476
C -2.525054 -1.198351 -0.735272
C -2.099471 -1.465893 0.740032
F -1.723882 -0.328093 1.351255
F -1.077769 -2.329111 0.771739
F -3.133498 -1.996896 1.422390
O -2.040826 -1.745861 -1.667064
Cl -3.845181 -0.017118 -0.846065
C 2.757828 -1.240784 -0.618198
C 2.412917 -1.146262 0.899242
F 1.319938 -0.377999 1.095657
F 3.435819 -0.607331 1.570399
F 2.165072 -2.372509 1.393762
O 3.817253 -0.949997 -1.064313
Cl 1.395978 -1.841137 -1.574891
C 0.164167 1.849070 -0.656270
C -0.280959 2.800127 0.495123

F 0.459249 2.571789 1.594313
F -1.568565 2.590166 0.786398
F -0.123888 4.084775 0.125399
O -0.536735 1.026311 -1.141209
Cl 1.845298 2.132127 -1.153695

E = -2733.664192
C -0.199492 2.049420 -0.211331
C 0.640669 2.053502 1.101514
F 1.904650 1.653057 0.857146
F 0.092861 1.226412 1.997231
F 0.677986 3.294175 1.620663
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M_4

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