

Electronic Supplementary Information

Is the regulation of the electronic properties of organic molecules by polynuclear superhalogens more effective than that by mononuclear superhalogens? A high-level *ab initio* case study

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Table S1. Calculated VDEs of the composite anions under study at various theoretical levels (in eV).

| | OVGF | CCSD | CCSD(T) |
|---|-------------------------|--------|---------|
| | AUG-CC-PVTZ | TZVP++ | |
| A | 5.52(0.91) ^a | 4.62 | 4.65 |
| B | 4.11(0.91) | 3.83 | 3.88 |
| C | 5.20(0.89) | 5.30 | 5.35 |
| A' | 5.81(0.90) | 4.88 | 4.90 |
| B' | 4.45(0.90) | 4.14 | 4.18 |
| C' | 5.42(0.89) | - | - |
| A1 | 6.20 (0.91) | 5.53 | 5.57 |
| A2 | 6.96(0.91) | 6.41 | 6.42 |
| A3 | 5.72(0.91) | 4.91 | 4.95 |
| A1' | 6.43(0.90) | 7.20 | 7.08 |
| A2' | 7.08(0.90) | 6.60 | 6.51 |
| A3' | 6.08(0.90) | 6.56 | 6.57 |
| B1 | 4.98(0.91) | 4.72 | 4.77 |
| B2 | 5.86(0.91) | 5.63 | 5.67 |
| B1' | 5.24(0.90) | 7.15 | 6.99 |
| B2' | 5.96(0.90) | 5.68 | 5.72 |
| C1 | 5.77(0.89) | - | - |
| C2 | 6.37(0.89) | 6.38 | 6.43 |
| C3 | 5.24(0.85) | - | - |
| C1' | 5.95(0.89) | 7.41 | 7.32 |
| C2' | 6.46(0.89) | - | - |
| C3' | 4.86(0.89) | - | - |
| Mg ₂ F ₅ (T) ^b | 7.43(0.86) | 8.92 | 8.82 |
| Mg ₂ F ₅ (D) ^c | 6.57(0.86) | 7.99 | 7.93 |
| Mg ₂ Cl ₅ (T) | 7.34(0.89) | 7.38 | 7.22 |
| Mg ₂ Cl ₅ (D) | 6.75(0.89) | 6.78 | 6.70 |
| MgF ₃ | 8.85(0.99) | 7.60 | 7.61 |
| MgCl ₃ | 6.72(0.91) | 6.37 | 6.23 |

^a Pole strength is shown in parenthesis.

^b Triple-bridge structure.

^c Double-bridge structure.

Point groups, lowest normal mode frequencies and optimized coordinates at MP2/6-311+G* level of the anions **A-A3**, **A'-A3'**, **B-B2**, **B'-B2'**, **C-C3**, **C'-C3'**.

A

Point group: Cs

Lowest normal mode frequency: 64.00 cm⁻¹ (A)

Optimized oordinates at MP2/6-311+G* level:

| | | | |
|----|-------------|-------------|----|
| C | 1.47356509 | -0.7682355 | 0. |
| H | 1.72949239 | -1.83947842 | 0. |
| C | 2.57131286 | 0.02999782 | 0. |
| H | 3.60365896 | -0.34273489 | 0. |
| H | 2.48372655 | 1.1178118 | 0. |
| Mg | -0.55406913 | -0.01779007 | 0. |
| F | -0.82598565 | 1.82297885 | 0. |
| F | -2.0003828 | -1.18883348 | 0. |

A'

Point group: Cs

Lowest normal mode frequency: 60.93 cm⁻¹ (A')

Optimized oordinates at MP2/6-311+G* level:

| | | | |
|----|-------------|-------------|----|
| C | 2.77029522 | -1.23862448 | 0. |
| H | 3.58747441 | -1.97004141 | 0. |
| H | 3.09305512 | -0.19646409 | 0. |
| C | 1.45535913 | -1.57190465 | 0. |
| H | 1.28328926 | -2.65840712 | 0. |
| Mg | -0.11327617 | -0.12440726 | 0. |
| Cl | -2.32517708 | -0.74122718 | 0. |
| Cl | 0.44526938 | 2.10481391 | 0. |

B

Point group: Cs

Lowest normal mode frequency: 21.02 cm⁻¹ (A'')

Optimized oordinates at MP2/6-311+G* level:

| | | | |
|----|---------------|---------------|---------------|
| C | 1.3617722512 | -0.8598793805 | 0. |
| H | 1.4553973009 | -1.5322115947 | 0.8695162292 |
| H | 1.4553973009 | -1.5322115947 | -0.8695162292 |
| C | 2.5497830616 | 0.1213985532 | 0. |
| H | 3.5393403425 | -0.366122385 | 0. |
| H | 2.5211631572 | 0.7806236216 | -0.8751892789 |
| H | 2.5211631572 | 0.7806236216 | 0.8751892789 |
| Mg | -0.6434904548 | -0.0085309054 | 0. |
| F | -0.8915776496 | 1.8401730604 | 0. |
| F | -2.1352214871 | -1.1283443566 | 0. |

B'

Point group: Cs

Lowest normal mode frequency: 8.64 cm⁻¹ (A'')

Optimized oordinates at MP2/6-311+G* level:

| | | | |
|----|---------------|---------------|---------------|
| C | 1.4049703898 | -0.8769777787 | 0. |
| H | 1.4993874264 | -1.5480504065 | 0.8697182361 |
| H | 1.4993874264 | -1.5480504065 | -0.8697182361 |
| C | 2.5832128325 | 0.1146562299 | 0. |
| H | 3.5732405435 | -0.3693195656 | 0. |
| H | 2.550483884 | 0.7728658394 | -0.8753698965 |
| H | 2.550483884 | 0.7728658394 | 0.8753698965 |
| Mg | -0.5786286671 | -0.043514827 | 0. |
| Cl | -0.9178429266 | 2.2367630701 | 0. |
| Cl | -2.4309678144 | -1.4157193559 | 0. |

C

Point group: Cs

Lowest normal mode frequency: 41.23 cm⁻¹ (A'')

Optimized oordinates at MP2/6-311+G* level:

| | | | |
|----|-------------|-------------|-------------|
| C | -0.00509979 | 1.0277178 | 1.19286123 |
| C | -0.00454682 | 2.43304778 | 1.20737102 |
| C | 0.02675 | 3.14303917 | 0. |
| C | -0.00454682 | 2.43304778 | -1.20737102 |
| C | -0.00509979 | 1.0277178 | -1.19286123 |
| C | -0.03567894 | 0.26223917 | 0. |
| H | -0.02200764 | 0.5093429 | 2.15382521 |
| H | 0.0189353 | 2.9723959 | 2.15536209 |
| H | 0.02740698 | 4.23288317 | 0. |
| H | 0.0189353 | 2.9723959 | -2.15536209 |
| H | -0.02200764 | 0.5093429 | -2.15382521 |
| Mg | -0.00489289 | -1.91198783 | 0. |
| F | 0.0113559 | -2.78984559 | -1.63454433 |
| F | 0.0113559 | -2.78984559 | 1.63454433 |

C'

Point group: Cs

Lowest normal mode frequency: 37.74 cm⁻¹ (A'')

Optimized oordinates at MP2/6-311+G* level:

| | | | |
|----|---------------|---------------|---------------|
| C | -0.0109790288 | 1.0516353312 | 1.1950007032 |
| C | -0.0041060917 | 2.456297032 | 1.2079162128 |
| C | 0.0300181071 | 3.1650873927 | 0. |
| C | -0.0041060917 | 2.456297032 | -1.2079162128 |
| C | -0.0109790288 | 1.0516353312 | -1.1950007032 |
| C | -0.0492069661 | 0.2915888402 | 0. |
| H | -0.0295786693 | 0.5320112538 | 2.1550166973 |
| H | 0.0228198069 | 2.996185858 | 2.1551561974 |
| H | 0.0367310695 | 4.254724544 | 0. |
| H | 0.0228198069 | 2.996185858 | -2.1551561974 |
| H | -0.0295786693 | 0.5320112538 | -2.1550166973 |
| Mg | -0.0050892702 | -1.8533552128 | 0. |
| Cl | 0.0210472427 | -2.9494067161 | -2.0081944837 |
| Cl | 0.0210472427 | -2.9494067161 | 2.0081944837 |

A1

Point group: Cs

Lowest normal mode frequency: 26.09 cm⁻¹ (A'')

Optimized oordinates at MP2/6-311+G* level:

| | | | |
|----|---------------|---------------|---------------|
| Mg | 1.6989188735 | 0.0752883348 | 0. |
| Mg | -0.8684172929 | -0.2410319416 | 0. |
| F | 3.5155797781 | 0.3012412101 | 0. |
| F | 0.2401062411 | 1.4132591127 | 0. |
| F | 0.5203582289 | -0.8328792101 | -1.3021038761 |
| F | 0.5203582289 | -0.8328792101 | 1.3021038761 |
| C | -2.9901061754 | -0.4527265528 | 0. |
| C | -3.8517945161 | 0.595218715 | 0. |
| H | -3.5092130432 | -1.4226466791 | 0. |
| H | -3.5035034045 | 1.6295266591 | 0. |
| H | -4.9422646831 | 0.4878858213 | 0. |

A1'

Point group: Cs

Lowest normal mode frequency: 26.81 cm⁻¹ (A'')

Optimized oordinates at MP2/6-311+G* level:

| | | | |
|----|---------------|---------------|---------------|
| Mg | 1.840304975 | 0.0797259237 | 0. |
| Mg | -1.0168606069 | -0.2702905068 | 0. |
| Cl | 4.0654769208 | 0.3617644362 | 0. |
| Cl | 0.1952123783 | 1.8578582045 | 0. |
| Cl | 0.5622761491 | -1.0746094848 | -1.6990294146 |
| Cl | 0.5622761491 | -1.0746094848 | 1.6990294146 |
| C | -3.1194411623 | -0.4634670675 | 0. |
| C | -3.9627995724 | 0.5985571033 | 0. |
| H | -3.6450729279 | -1.4286451905 | 0. |
| H | -3.5971725422 | 1.6266396383 | 0. |
| H | -5.0541775311 | 0.5073326884 | 0. |

A2

Point group: Cs

Lowest normal mode frequency: 23.62 cm⁻¹ (A'')

Optimized oordinates at MP2/6-311+G* level:

| | | | |
|----|---------------|---------------|---------------|
| Mg | 0.0700208605 | 1.7594818364 | 0. |
| Mg | -0.2650574955 | -1.1586044901 | 0. |
| F | 1.1826823644 | 0.0547055016 | 0. |
| F | -1.399617141 | 0.351441042 | 0. |
| F | 0.1604837263 | 2.5604525636 | 1.6670408574 |
| F | 0.1604837263 | 2.5604525636 | -1.6670408574 |
| C | -0.4775810607 | -3.2607566303 | 0. |
| H | -1.4473148568 | -3.7755325101 | 0. |
| C | 0.5785576017 | -4.1111670793 | 0. |
| H | 1.6098620745 | -3.7561906902 | 0. |
| H | 0.4761912476 | -5.2007801833 | 0. |

A2'

Point group: Cs

Lowest normal mode frequency: 8.33 cm⁻¹ (A'')

Optimized oordinates at MP2/6-311+G* level:

| | | | |
|----|---------------|---------------|---------------|
| Mg | 0.0870161594 | 1.9773767559 | 0. |
| Mg | -0.3223731936 | -1.3478313937 | 0. |
| Cl | 1.587877723 | -0.0234095562 | 0. |
| Cl | -1.8538637582 | 0.3965731 | 0. |
| Cl | 0.2015891084 | 2.9553861316 | 2.0452066998 |
| Cl | 0.2015891084 | 2.9553861316 | -2.0452066998 |
| C | -0.5005826043 | -3.4416956714 | 0. |
| H | -1.4558620096 | -3.9813930637 | 0. |
| C | 0.5836171864 | -4.2556320752 | 0. |
| H | 1.6018265667 | -3.8646638604 | 0. |
| H | 0.5179447011 | -5.3478668137 | 0. |

A3

Point group: Cs

Lowest normal mode frequency: 14.56 cm⁻¹ (A')

Optimized oordinates at MP2/6-311+G* level:

| | | | |
|----|-----------------|-----------------|-----------------|
| Mg | -0.323094000000 | -1.963802000000 | 0.000000000000 |
| Mg | -0.077460000000 | 0.958436000000 | 0.000000000000 |
| F | -0.077460000000 | -0.634818000000 | 1.300707000000 |
| F | -0.077460000000 | -0.634818000000 | -1.300707000000 |
| F | -0.563989000000 | -3.763786000000 | 0.000000000000 |
| F | -1.825789000000 | 1.587950000000 | 0.000000000000 |
| C | 1.748334000000 | 2.099594000000 | 0.000000000000 |
| C | 1.804824000000 | 3.455708000000 | 0.000000000000 |
| H | 2.751412000000 | 1.643188000000 | 0.000000000000 |
| H | 0.900359000000 | 4.066841000000 | 0.000000000000 |
| H | 2.738198000000 | 4.031807000000 | 0.000000000000 |

A3'

Point group: Cs

Lowest normal mode frequency: 11.38 cm⁻¹ (A')

Optimized oordinates at MP2/6-311+G* level:

| | | | |
|----|---------------|---------------|---------------|
| Mg | -0.3139701901 | -2.189252592 | 0. |
| Mg | -0.062334628 | 1.1532593873 | 0. |
| Cl | -0.0122121708 | -0.7184535151 | 1.7372346289 |
| Cl | -0.0122121708 | -0.7184535151 | -1.7372346289 |
| Cl | -0.6451078449 | -4.3903841831 | 0. |
| Cl | -2.222928981 | 1.8967995705 | 0. |
| C | 1.7746774741 | 2.2171726722 | 0. |
| C | 1.8872854777 | 3.5687392442 | 0. |
| H | 2.7498700133 | 1.707153035 | 0. |
| H | 1.0100609599 | 4.2178447182 | 0. |
| H | 2.8447420575 | 4.1018751759 | 0. |

B1

Point group: Cs

Lowest normal mode frequency: 11.86 cm⁻¹ (A'')

Optimized oordinates at MP2/6-311+G* level:

| | | | |
|----|---------------|---------------|---------------|
| Mg | -1.7906459892 | 0.0881040164 | 0. |
| Mg | 0.7749789463 | -0.2750633482 | 0. |
| F | -3.6046035986 | 0.3411946079 | 0. |
| F | -0.4205564705 | 0.6560273922 | 1.3055717049 |
| F | -0.7358205191 | -1.5839444387 | 0. |
| F | -0.4205564705 | 0.6560273922 | -1.3055717049 |
| C | 2.900922398 | -0.5693011749 | 0. |
| H | 3.177339289 | -1.1848341002 | 0.8712775908 |
| H | 3.177339289 | -1.1848341002 | -0.8712775908 |
| C | 3.7752330228 | 0.7017216624 | 0. |
| H | 4.8570144046 | 0.4957169471 | 0. |
| H | 3.5736174165 | 1.3261766878 | 0.8780224255 |
| H | 3.5736174165 | 1.3261766878 | -0.8780224255 |

B1'

Point group: Cs

Lowest normal mode frequency: 21.45 cm⁻¹ (A'')

Optimized oordinates at MP2/6-311+G* level:

| | | | |
|----|---------------|---------------|---------------|
| Mg | -1.9337469397 | 0.111342869 | 0. |
| Mg | 0.9160426629 | -0.3415646691 | 0. |
| Cl | -4.1535223173 | 0.448037679 | 0. |
| Cl | -0.3938589802 | 0.8639514814 | 1.7041125947 |
| Cl | -0.8496486706 | -2.0520234456 | 0. |
| Cl | -0.3938589802 | 0.8639514814 | -1.7041125947 |
| C | 3.0252244368 | -0.6017593221 | 0. |
| H | 3.3223339675 | -1.2038993932 | 0.8727660547 |
| H | 3.3223339675 | -1.2038993932 | -0.8727660547 |
| C | 3.8370014345 | 0.7096573551 | 0. |
| H | 4.9261507748 | 0.5521328428 | 0. |
| H | 3.6067138946 | 1.3236203691 | 0.878127908 |
| H | 3.6067138946 | 1.3236203691 | -0.878127908 |

B2

Point group: Cs

Lowest normal mode frequency: 18.15 cm⁻¹ (A'')

Optimized oordinates at MP2/6-311+G* level:

| | | | |
|----|---------------|---------------|---------------|
| Mg | -1.8637384893 | -0.0000000268 | 0.0803943259 |
| Mg | 1.0538053878 | -0.0000000052 | -0.2977078049 |
| F | -2.6689429858 | 1.6655905742 | 0.1840637278 |
| F | -0.1470751119 | -0.0000000141 | 1.1669576996 |
| F | -2.668942961 | -1.6655906398 | 0.1840637278 |
| F | -0.4802593216 | -0.0000000166 | -1.4077998927 |
| C | 3.1683709255 | 0.0000000106 | -0.575558619 |
| H | 3.4392705468 | 0.8699228914 | -1.1934940837 |
| H | 3.4392705597 | -0.8699228663 | -1.1934940837 |
| C | 4.0408475118 | 0.000000017 | 0.6957603055 |
| H | 3.842449833 | -0.8772866713 | 1.3207961314 |
| H | 3.8424498199 | 0.8772867024 | 1.3207961314 |
| H | 5.1189153979 | 0.000000025 | 0.4796634336 |

B2'

Point group: Cs

Lowest normal mode frequency: 5.64 cm⁻¹ (A'')

Optimized oordinates at MP2/6-311+G* level:

| | | | |
|----|---------------|---------------|---------------|
| Mg | -2.1176084973 | -0.0000000287 | 0.0933397181 |
| Mg | 1.2194675793 | -0.000000004 | -0.3328774104 |
| Cl | -3.1016626071 | 2.0434931819 | 0.2181387697 |
| Cl | -0.1117301406 | -0.0000000138 | 1.58132167 |
| Cl | -3.1016625768 | -2.0434932539 | 0.2181387697 |
| Cl | -0.5504337299 | -0.0000000171 | -1.8493765645 |
| C | 3.3261118619 | 0.0000000117 | -0.5915019804 |
| H | 3.6053385274 | 0.8701501858 | -1.2048779477 |
| H | 3.6053385403 | -0.8701501583 | -1.2048779477 |
| C | 4.1710924522 | 0.0000000179 | 0.6975625234 |
| H | 3.9596179593 | -0.8772505918 | 1.3181511084 |
| H | 3.9596179463 | 0.8772506246 | 1.3181511084 |
| H | 5.2529337936 | 0.000000026 | 0.5031491819 |

C1

Point group: C1

Lowest normal mode frequency: 10.84 cm⁻¹ (A)

Optimized oordinates at MP2/6-311+G* level:

| | | | |
|----|---------------|---------------|---------------|
| Mg | -0.0366885974 | -0.0334565403 | -0.4690671125 |
| Mg | 0.0696694406 | -0.0101533372 | -3.0478549386 |
| F | -0.8634317644 | 1.1996548918 | -1.7877073453 |
| F | 1.5145141778 | 0.1245180025 | -1.6956595762 |
| F | -0.6122488167 | -1.3891529217 | -1.8014022287 |
| F | 0.1520380832 | 0.0068878913 | -4.8747625852 |
| C | -0.0410703099 | -0.0407941783 | 1.6770168473 |
| C | 1.1553543008 | 0.1438384805 | 2.4153409459 |
| C | 1.1958785718 | 0.178660161 | 3.8189674321 |
| C | 0.0079519392 | 0.080844651 | 4.5534688864 |
| C | -1.2010358613 | -0.1032801376 | 3.8713769404 |
| C | -1.2140816252 | -0.1343348351 | 2.4673666223 |
| H | 2.1055647784 | 0.2296594507 | 1.8839509718 |
| H | 2.1450107862 | 0.321754445 | 4.3359551309 |
| H | 0.0285092927 | 0.1075669892 | 5.6422536465 |
| H | -2.1343458193 | -0.1810215346 | 4.4294881424 |
| H | -2.1811699063 | -0.2737904581 | 1.9794150806 |

C1'

Point group: Cs

Lowest normal mode frequency: 10.28 cm⁻¹ (A'')

Optimized oordinates at MP2/6-311+G* level:

| | | | |
|----|---------------|---------------|---------------|
| Mg | 0.0216980662 | -0.0266271839 | -0.3645167068 |
| Mg | 0.0324044005 | -0.0175003025 | -3.2308393192 |
| Cl | -0.5154914166 | 1.8686967704 | -1.8196476675 |
| Cl | 1.9373394152 | -0.4849924995 | -1.800430443 |
| Cl | -1.3470035709 | -1.427499969 | -1.8144164074 |
| Cl | 0.0470015455 | -0.0363359373 | -5.4718748294 |
| C | 0.0172969898 | -0.0362342778 | 1.7567318518 |
| C | 1.1521970281 | 0.3320378484 | 2.520447628 |
| C | 1.1483169351 | 0.3766753075 | 3.9237445434 |
| C | -0.0263523472 | 0.083316473 | 4.6272331489 |
| C | -1.1740550283 | -0.288051 | 3.9161303482 |
| C | -1.1452007441 | -0.3255287763 | 2.5129134184 |
| H | 2.0892354907 | 0.5683776158 | 2.0119299271 |
| H | 2.0492058344 | 0.6655301653 | 4.465090202 |
| H | -0.0392626605 | 0.1159426236 | 5.7158193008 |
| H | -2.0946164983 | -0.5205178211 | 4.451495409 |
| H | -2.0622947694 | -0.6198880166 | 1.9983364559 |

C2

Point group: Cs

Lowest normal mode frequency: 18.86 cm⁻¹ (A')

Optimized oordinates at MP2/6-311+G* level:

| | | | |
|----|---------------|---------------|---------------|
| Mg | -0.0243952367 | 3.1551330373 | 0. |
| Mg | 0.0254538907 | 0.2248292526 | 0. |
| F | -0.0036977735 | 1.5860112288 | -1.3024876505 |
| F | -0.0036977735 | 1.5860112288 | 1.3024876505 |
| F | -1.7020881766 | 3.9348818774 | 0. |
| F | 1.6380514627 | 3.9675426126 | 0. |
| C | 0.0237719021 | -2.6596775076 | 1.1964604036 |
| C | 0.0075361998 | -4.0632265571 | 1.207783447 |
| C | -0.0274008645 | -4.7702530399 | 0. |
| C | 0.0075361998 | -4.0632265571 | -1.207783447 |
| C | 0.0237719021 | -2.6596775076 | -1.1964604036 |
| C | 0.0606368199 | -1.9012600974 | 0. |
| H | 0.0453556707 | -2.1486119117 | 2.160699768 |
| H | -0.0191494832 | -4.6015638799 | 2.1547532988 |
| H | -0.04209336 | -5.8590465104 | 0. |
| H | -0.0191494832 | -4.6015638799 | -2.1547532988 |
| H | 0.0453556707 | -2.1486119117 | -2.160699768 |

C2'

Point group: Cs

Lowest normal mode frequency: 4.44 cm⁻¹ (A')

Optimized oordinates at MP2/6-311+G* level:

| | | | |
|----|---------------|---------------|---------------|
| Mg | -0.0220120888 | 3.4374331312 | 0. |
| Mg | 0.0172605324 | 0.1025953806 | 0. |
| Cl | -0.013824221 | 1.6296639826 | -1.7403069303 |
| Cl | -0.013824221 | 1.6296639826 | 1.7403069303 |
| Cl | -2.07124337 | 4.4071659652 | 0. |
| Cl | 2.0254410944 | 4.4123557378 | 0. |
| C | 0.0167789045 | -2.7657106413 | 1.1974519729 |
| C | 0.0121504731 | -4.169065401 | 1.2083052355 |
| C | -0.0174335098 | -4.8757482674 | 0. |
| C | 0.0121504731 | -4.169065401 | -1.2083052355 |
| C | 0.0167789045 | -2.7657106413 | -1.1974519729 |
| C | 0.0460893096 | -2.0099191634 | 0. |
| H | 0.0347623462 | -2.2523837386 | 2.1606067941 |
| H | -0.00930809 | -4.7083210146 | 2.1547832014 |
| H | -0.0234232277 | -5.9645592322 | 0. |
| H | -0.00930809 | -4.7083210146 | -2.1547832014 |
| H | 0.0347623462 | -2.2523837386 | -2.1606067941 |

C3

Point group: C1

Lowest normal mode frequency: 12.11 cm⁻¹ (A)

Optimized oordinates at MP2/6-311+G* level:

| | | | |
|----|---------------|---------------|---------------|
| Mg | -0.1507584291 | -0.6405775294 | -1.0894228744 |
| Mg | 2.027371369 | 0.1823839225 | 0.6983200976 |
| F | 1.2091624263 | 0.8682887581 | -0.8498162336 |
| F | 0.8678324826 | -1.286629654 | 0.5649758376 |
| F | 3.3688158367 | 0.7099581199 | 1.7987519504 |
| F | 0.2461803811 | -1.7392407021 | -2.5215288846 |
| C | -4.4476347441 | 0.0906952959 | 0.1755693958 |
| C | -3.2642030977 | -0.4920280507 | -0.3084208517 |
| C | -2.0431518944 | 0.2153032562 | -0.446844497 |
| C | -2.1012848043 | 1.5665451086 | -0.0178998717 |
| C | -3.2696327198 | 2.1762758444 | 0.4708220089 |
| C | -4.4471807351 | 1.4282366436 | 0.5915955785 |
| H | -5.357840248 | -0.5044219268 | 0.2595721226 |
| H | -3.3132415148 | -1.5382921359 | -0.6189874289 |
| H | -1.2070254722 | 2.1886336046 | -0.1005433486 |
| H | -3.2540881217 | 3.2207910761 | 0.7847925368 |
| H | -5.3591451245 | 1.8899461189 | 0.9689389525 |

C3'

Point group: C1

Lowest normal mode frequency: 7.08 cm⁻¹ (A)

Optimized oordinates at MP2/6-311+G* level:

| | | | |
|----|---------------|---------------|---------------|
| Mg | -0.319062342 | -0.7520674128 | -0.863164656 |
| Mg | 2.5289091325 | 0.3503182639 | 0.539685468 |
| Cl | 1.4133749127 | 1.0236668388 | -1.3571852097 |
| Cl | 0.9975506631 | -1.1969324623 | 1.266070971 |
| Cl | 4.4567478133 | 1.0457354555 | 1.4014291167 |
| Cl | -0.0070687564 | -2.5424557494 | -2.2334291244 |
| C | -4.6193788104 | 0.1900850037 | -0.113106381 |
| C | -3.409615005 | -0.4060112262 | -0.5057787967 |
| C | -2.1501403643 | 0.2256594035 | -0.3565738107 |
| C | -2.1935005187 | 1.4949702605 | 0.270838239 |
| C | -3.3886687038 | 2.1150325414 | 0.6697553117 |
| C | -4.6087886795 | 1.4475485976 | 0.5032252266 |
| H | -5.5622993039 | -0.3393492659 | -0.2525776536 |
| H | -3.4617432141 | -1.3870826075 | -0.982655048 |
| H | -1.2650274779 | 2.0519594804 | 0.4168422872 |
| H | -3.3657343426 | 3.0961807983 | 1.1448180794 |
| H | -5.5413794131 | 1.9186098305 | 0.8116804706 |