Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

The [2+2] Cycloaddition Product of Perhalogenated Cyclopentadienyl Cations: Structural Characterization of Salts of the $[C_{10}Cl_{10}]^{2+}$ and $[C_{10}Br_{10}]^{2+}$ Dications

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Content

1 Experimental Part

1.1 General Procedures

Commercially available chemicals were used as received, unless otherwise noted. AsF_5 [1] and C_5Br_6 [2] were prepared as described previously in the literature. SbF_5 was stored inside a glove box. SbF_5 and AsF_5 are highly dangerous compounds with devastating effects on human tissue. They should only be handled in appropriate equipment by trained personnel. Attention: AsF_5, SO_2 and SO_2ClF are (toxic) gases at room temperature. C_5Cl_6 was purchased from ABCR. Oxygen- and moisture-sensitive compounds were handled using Schlenk techniques and/or handled and stored in a argon-filled glovebox ($O_{2(g)}$ and $H_2O_{(g)} < 0.1$ ppm). SO_2 was distilled from CaH_2 and stored in a stainless-steel cylinder. SO_2ClF was prepared according to literature methods[3] and stored in a stainless-steel cylinder. Reactions involving SO_2ClF, AsF_5 and SbF_5 were performed in PFA (tetrafluoroethene-perfluoroalkoxyvinyl-copolymer) tubes connected to stainless-steel valves. Instead of stirring, the mixtures were agitated with the help of the Mini-Vortex Mixer PV-1.

^{13}C and ^{19}F NMR spectra were recorded on a JEOL 400 MHz ECS spectrometer by using sealed 5mm PFA tubes inside 6mm NMR glass tubes containing d_6-acetone as external lock standard. All reported chemical shifts (δ) are referenced to the Ξ values given in IUPAC recommendations of 2008 using the ^2H signal of the deuterated solvent as internal reference.[4] All chemical shifts (δ) are given in parts per million (ppm) and the signals are specified according to the multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet, br = broad) and the coupling constants *J* in Hz.

X-Ray data were collected on a BRUKER D8 Venture system. Data were collected at 100(2) K using graphite-monochromated Mo K_α radiation (λ_α = 0.71073 Å). The strategy for the data collection was evaluated by using the Smart software. The data were collected by the standard "ψ-ω scan techniques" and were scaled and reduced using Saint+software. The structures were solved by using Olex2,[5] the structure was solved with the XT [6] structure solution program using Intrinsic Phasing and refined with the XL [7] refinement package using Least Squares minimization. If it is noted, bond length and angles were measured with Diamond Crystal and Molecular Structure Visualization Version 3.1. [8] Drawings were generated with Mercury.[9]

1.2 Synthesis

C_5Cl_6:

C_5Cl_6 (30 mg) was filled into a 8 mm PFA tube equipped with a stainless steel valve. SO_2 (0.5 mL) was condensed in at -196 °C. The C_5Cl_6 was dissolved at -20 °C. Afterwards, 0.4 mL of the solvent was evaporated under high vacuum. The mixture was slowly cooled to -78 °C in a freezer. The next day, colorless single crystals of C_5Cl_6 had formed.

^{13}C NMR (100 MHz, CH_2Cl_2, ex. acetone-d_6, r.t.): δ = 131.49, 128.01, 88.66 ppm.

C_5Br_6:

KOH (220 g, 3.93 mol) was dissolved in 700 mL deionized water while stirring vigorously. Then bromine (30 mL, 0.59 mol) was added to the solution dropwise at 0 °C. Afterwards, the yellow solution was

warmed up to room temperature. After addition of freshly distilled cyclopentadiene (5 g, 0.08 mol) in 5 mL pentane a colorless precipitate had formed. The color changed from colorless to brown while stirring over night at room temperature. The brown precipitate was filtered off, washed with deionized water and dissolved in pentane. The solution was dried over $MgSO_4$, purified over active carbon and filtered. During the evaporation of the solvent at ambient pressure, brown crystals formed. The crystalline residue was washed with small amounts of pentane and recrystallized two times in methanol at reflux. After cooling down to room temperature C_5Br_6 was isolated as yellow crystalline solid in 47% yield (20 g, 0.04 mol). C_5Br_6 (50 mg) was dissolved in a mixture of dichloromethane (2 mL) and acetonitrile (0.5 mL). The mixture was slowly cooled to -78 °C in a freezer. After three months yellow single crystals of C_5Br_6 · MeCN had formed.

^{13}C NMR (100 MHz, CD_2Cl_2, r.t.): δ = 130.21, 122.97, 56.96 ppm.

$[C_{10}Cl_{10}][Sb_3F_{16}]_2$:

Inside a glovebox, antimony pentafluoride (1 g, 4.61 mmol) was filled into a 8 mm PFA tube equipped with a stainless steel valve. SO_2ClF (1 mL) was condensed in at -196°C. After the antimony pentafluoride was dissolved at -20°C, the mixture was frozen again. Subsequently, C_5Cl_6 (0.1 g, 0.37 mmol) was added to the frozen solution. The mixture was brought to -20 °C, resulting in a green solution. The mixture was slowly cooled to -78 °C in a freezer. The next day, moisture-sensitive, thermally unstable yellow single crystals of $[C_{10}Cl_{10}][Sb_3F_{16}]_2$ · 2 SO_2ClF had formed in the green solution.

^{13}C NMR (100 MHz, SO_2, ext. acetone-d_6, -60 °C): δ = 219.08, 158.23, 76.05 ppm.

^{19}F NMR (377 MHz, SO_2, ext. acetone-d_6, -60 °C): δ = -91.37 (br, 1F), -101.4 (br, 5F), -110.57 (br, 7F), 132.66 (br, 2F), -134.22 (br, 1F) ppm.

$[C_{10}Br_{10}][As_2F_{11}]_2$:

C_5Br_6 (40 mg, 0.07 mmol) was filled into a 8 mm PFA tube equipped with a stainless steel valve. SO_2ClF (1 mL) was condensed in at -196°C. Subsequently, AsF_5 (25 mg, 0.15 mmol) was condensed to the frozen solution. The mixture was brought to -20 °C, resulting in a dark orange solution. The mixture was slowly cooled to -78 °C in a freezer. The next day, moisture-sensitive, thermally unstable orange single crystals of $[C_{10}Br_{10}][As_2F_{11}]_2$ · 4 SO_2ClF had formed in the green solution.

^{13}C NMR (100 MHz, SO_2, ext. acetone-d_6, -60 °C): δ = 219.32, 155.29, 68.27 ppm.

^{19}F NMR (377 MHz, SO_2, ext. acetone-d_6, -60 °C): δ = -56.06 (br) ppm.

2 Appendix

2.1 Crystallographic data

Table S1: *Crystallographic Data*

Compound	**$[C_{10}Cl_{10}][Sb_3F_{16}]_2 \cdot 2\ SO_2ClF$**	**$[C_{10}Br_{10}][As_2F_{11}]_2 \cdot 4\ SO_2ClF$**
Empirical formula	$C_{10}Cl_{12}F_{34}O_4S_2Sb_6$	$As_4Br_{10}C_{10}Cl_4F_{26}O_8S_4$
Formula weight	2050.12	2110.92
Temperature/K	102.37	100.09
Crystal system	Monoclinic	triclinic
Space group	$P2_1/n$	P-1
a/Å	9.8021(4)	8.8126(5)
b/Å	19.9917(8)	11.9355(8)
c/Å	12.0793(5)	12.5355(8)
α/°	90	68.761(2)
β/°	97.4060(10)	74.151(2)
γ/°	90	75.960(2)
Volume/Å³	2347.32(17)	1166.97(13)
Z	2	1
ρ_{calc}/g·cm³	2.901	3.004
μ/mm^{-1}	4.338	11.948
F(000)	1880.0	972.0
Crystal size/mm³	0.347 × 0.255 × 0.222	0.152 × 0.125 × 0.098
Crystal shape	block	plate
Radiation	MoK_α (λ = 0.71073)	MoK_α (λ = 0.71073)
2Θ range for data collection/°	4.66 to 56.692	4.868 to 52.886
Index ranges	-11 ≤ h ≤ 13, -26 ≤ k ≤ 26, -16 ≤ l ≤ 16	-11 ≤ h ≤ 11, -14 ≤ k ≤ 14, -15 ≤ l ≤ 15
Reflections collected	93745	80540
Independent reflections	5828 [R_{int} = 0.0451, R_{sigma} = 0.0157]	4806 [R_{int} = 0.0568, R_{sigma} = 0.0198]
Data/restrains/parameters	5828/0/326	4806/0/326
Goodness-of-fit on F²	1.131	0.987
Final R indexes [I>=2σ(I)]	R_1 = 0.0173, wR_2 = 0.0408	R_1 = 0.0283, wR_2 = 0.0601
Final R indexes [all data]	R_1 = 0.0183, wR_2 = 0.0411	R_1 = 0.0319, wR_2 = 0.0617
Largest diff. peak/hole / e·Å³	0.78/-0.78	1.34/-0.78

Table S2: *Crystallographic Data*

Compound	**C_5Cl_6**	**C_5Br_6 · MeCN**
Empirical formula	C_5Cl_6	$C_7H_3Br_6N$
Formula weight	272.75	580.56
Temperature/K	100.0	103.68
Crystal system	Triclinic	orthorhombic
Space group	P-1	Pnma
a/Å	8.2289(4)	8.5108(5)
b/Å	10.3003(5)	7.1691(4)
c/Å	12.5070(6)	21.9711(11)
α/°	97.189(2)	90
β/°	107.491(2)	90
γ/°	111.379(2)	90
Volume/Å³	908.04(8)	1340.56(13)
Z	4	4
ρ_{calc}/g·cm³	1.995	2.877
μ/mm^{-1}	1.817	17.933
F(000)	528.0	1048.0
Crystal size/mm³	0.504 × 0.386 × 0.201	0.531 × 0.179 × 0.16
Crystal shape	block	block
Radiation	MoK_α (λ = 0.71073)	MoK_α (λ = 0.71073)
2Θ range for data collection/°	4.404 to 56.656	5.132 to 51.386
Index ranges	-10 ≤ h ≤ 10, -13 ≤ k ≤ 13, -16 ≤ l ≤ 16	-10 ≤ h ≤ 10, -8 ≤ k ≤ 8, -26 ≤ l ≤ 26
Reflections collected	31668	21875
Independent reflections	4500 [R_{int} = 0.0275, R_{sigma} = 0.0171]	1385 [R_{int} = 0.0661, R_{sigma} = 0.0277]
Data/restrains/parameters	4500/0/199	1385/0/84
Goodness-of-fit on F²	1.056	1.080
Final R indexes [I>=2σ(I)]	R_1 = 0.0206, wR_2 = 0.0515	R_1 = 0.0474, wR_2 = 0.1380
Final R indexes [all data]	R_1 = 0.0244, wR_2 = 0.0541	R_1 = 0.0491, wR_2 = 0.1392
Largest diff. peak/hole / e·Å³	0.50/-0.30	1.15/-1.61

The solid state structure of **1a** contains two independent C_5Cl_6 molecules in the asymmetric unit. The differences in bond distances and angles of both molecules are equal within ± 3σ. In structure of **1b · MeCN** the cyclopentadienyl ring is located in a crystallographic mirror plane. All atoms in this plane have a side occupation factor of 0.5 yielding an overall formula of C_5Br_6. In both compounds C1 is a saturated carbon atom. The C-C and C-X distances (X = Cl, Br) in these positions equals normal single bonds. The other C-C bond lengths (C2 to C5) exhibit a conjugated double bond system with distances of 1.34 and 1.48 Å. The halogen atoms attached to these carbon atoms contribute to the conjugated system. As a result, the C-Cl distances are decreased by 0.08 Å compared to the C_{sp_3}-X lengths in the crystal structure of **1a** and **1b**. Additionally, the crystal structure of **1a** shows short Cl···Cl contacts (3.334(3) to 3.493(3) Å) connecting each C_5Cl_6 unit in a polymeric structure. In the

structure of **1b · MeCN** the halogen bonds are replaced by solvent interactions (N-Br distance: 2.977(17) Å).

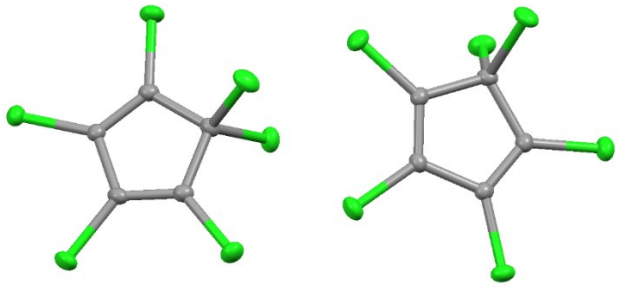

Figure S1: *Ellipsoid (50% prob.) plot of compound C_5Cl_6. Color code: green – chlorine, grey – carbon.*

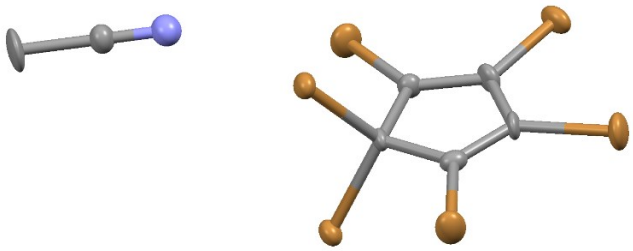

Figure S2: *Ellipsoid (50% prob.) plot of compound C_5Br_6 · MeCN. Hydrogen atoms are omitted for clarity. Color code: blue – nitrogen, orange – bromine, grey – carbon.*

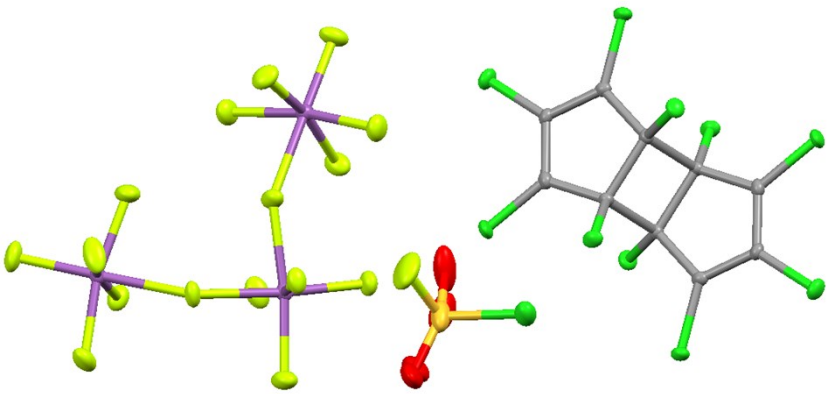

Figure S3: *Ellipsoid (50% prob.) plot of compound $[C_{10}Cl_{10}][Sb_3F_{16}]_2$ · SO_2ClF. Color code: purple – antimony, green – chlorine, dark yellow – sulfur, yellow – fluorine, red – oxygen, grey – carbon.*

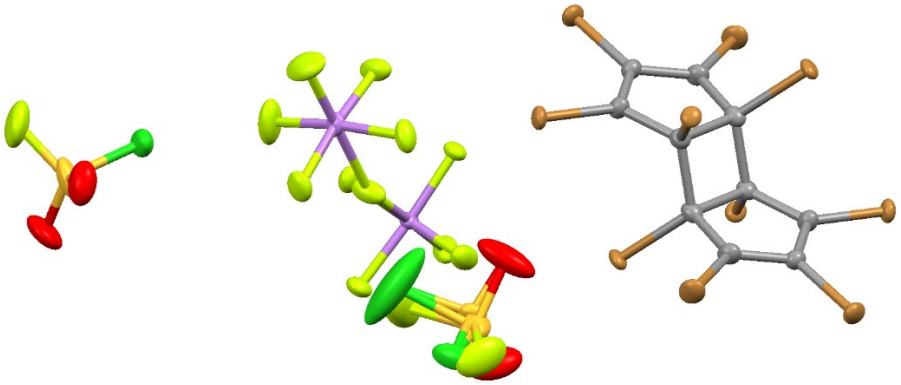

Figure S4: *Ellipsoid (50% prob.) plot of compound* $[C_{10}Br_{10}][As_2F_{11}]_2 \cdot 2\ SO_2ClF$. *Color code: violet – arsenic, orange – bromine, green – chlorine, dark yellow – sulfur, yellow – fluorine, red – oxygen, grey – carbon.*

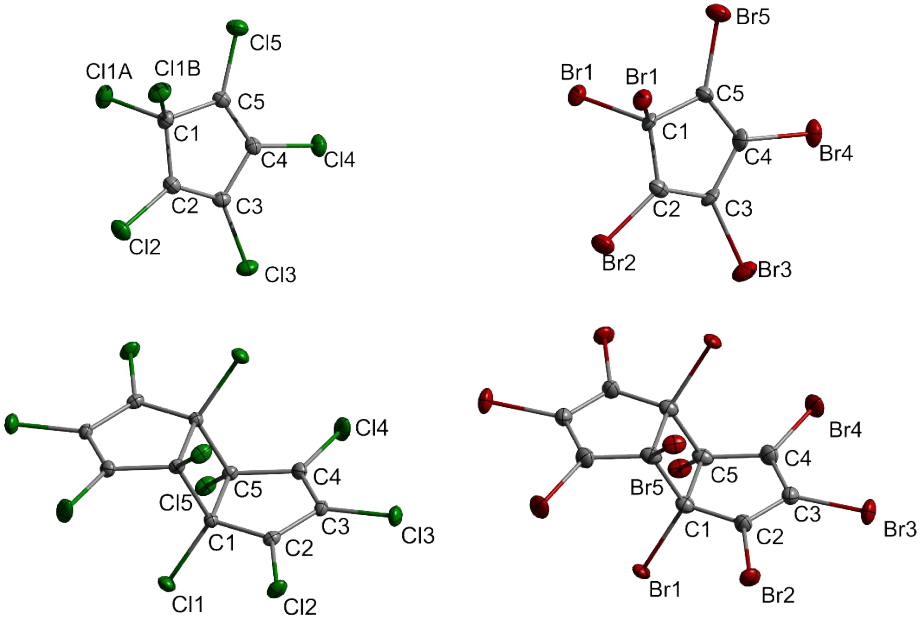

Figure S5: *Ellipsoid (50% prob.) plot of compounds* ***1a***, ***1b*** $\cdot$ ***MeCN***, $[\mathbf{4a}][Sb_3F_{16}]_2 \cdot SO_2ClF$ *(left) and* $[\mathbf{4b}][As_2F_{11}]_2 \cdot 2\ SO_2ClF$ *(right). Counterions and solvent molecules are omitted for clarity. Color code: red – bromine, green – chlorine, grey – carbon.*

Table S3: *Selected bond lengths of the compounds* ***1a***, ***1b***, $[\mathbf{4a}][Sb_3F_{16}]_2$ *and* $[\mathbf{4b}][As_2F_{11}]_2$ *[Å]*

	$(C_{10}X_{10})^{2+}$		C_5X_6	
	X = Cl	**X = Br**	**X = Cl**	**X = Br**
C1 – C2	1.507(3)	1.501(7)	1.511(3)	1.509(15)
C2 – C3	1.386(3)	1.386(6)	1.336(2)	1.311(15)
C3 – C4	1.394(3)	1.392(8)	1.475(2)	1.470(16)
C4 – C5	1.507(3)	1.511(6)	1.334(3)	1.365(15)
C5 – C1	1.566(3)	1.568(7)	1.507(2)	1.505(14)
C1 – X1	1.740(2)	1.908(4)	1.781(2),1.780(2)	1.950(6)
C2 – X2	1.643(2)	1.803(6)	1.696(1)	1.856(10)
C3 – X3	1.678(2)	1.833(5)	1.698(2)	1.875(11)
C4 – X4	1.634(2)	1.797(4)	1.697(1)	1.840(11)
C5 – X5	1.739(2)	1.912(5)	1.699(2)	1.838(11)

2.2 NMR spectra

The samples of the dications were prepared in sealed 5 mm PFA tubes. The mother liquor was decanted off and the remaining single-crystals were dissolved in cold SO_2. The tubes were resealed in vacuum and stored in cold ethanol at -75°C. For the measurement, they were taken out, rapidly wiped off and placed inside a 6mm glass NMR tube containing acetone-d_6. Therefore, signals of acetone and ethanol can be observed in the ^{13}C NMR spectra.

$[C_{10}Br_{10}][As_2F_{11}]_2$:

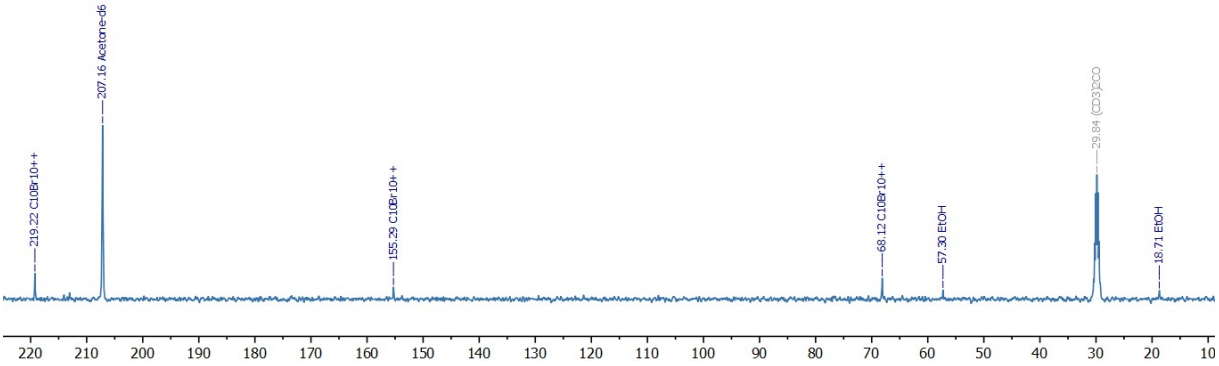

Figure S6: *^{13}C NMR spectrum (100 MHz, SO_2, ext. acetone-d_6, -60 °C).*

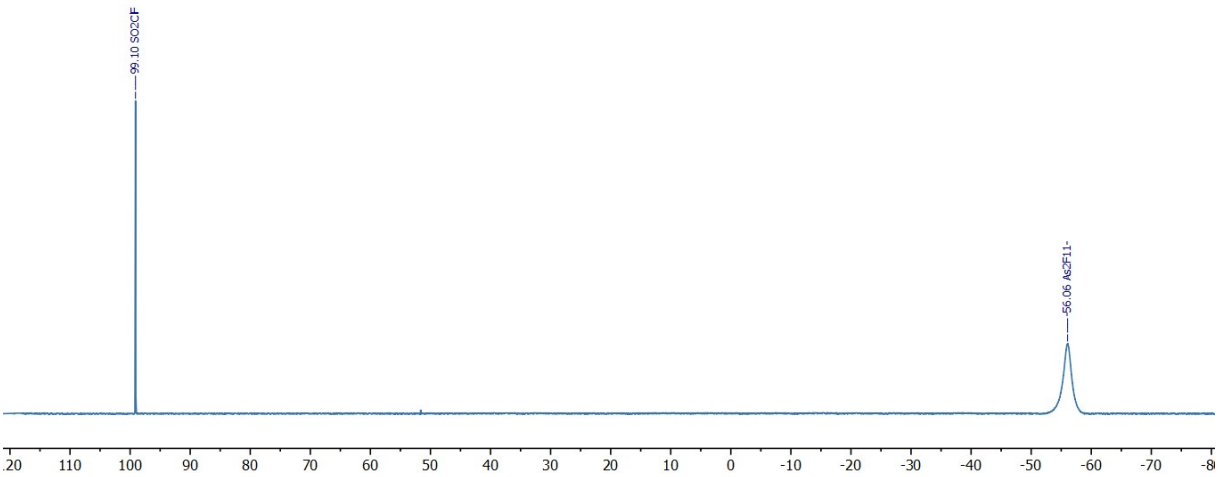

Figure S7: *^{19}F NMR spectrum (377 MHz, SO_2, ext. acetone-d_6, -60 °C).*

In case of $[C_{10}Br_{10}]^{2+}$ the NMR sample was warmed to -20°C as well (spectra below). The signals which we assigned to the dication vanish and new signals at 212 and 127 ppm appear as well as the formation of a brown oil was observed. The decomposition products are not identified yet.

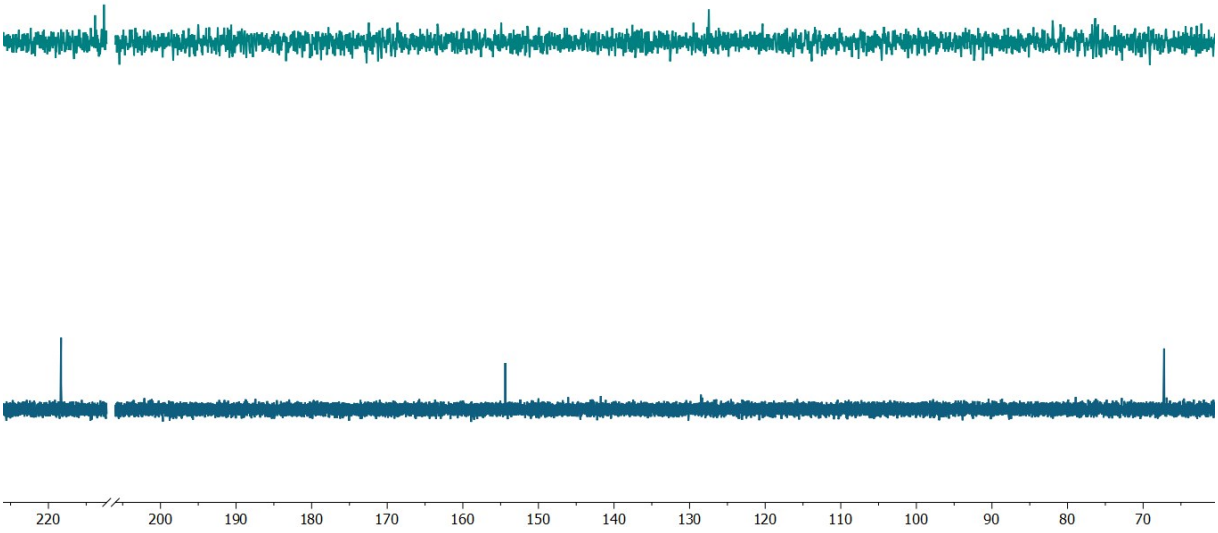

Figure S8: *^{13}C NMR spectra (100 MHz, SO_2, ext. acetone-d_6) of $[C_{10}Br_{10}][As_2F_{11}]_2$ at first at -60°C (bottom) and afterwards at -20°C (top).*

$[C_{10}Cl_{10}][Sb_3F_{16}]_2$:

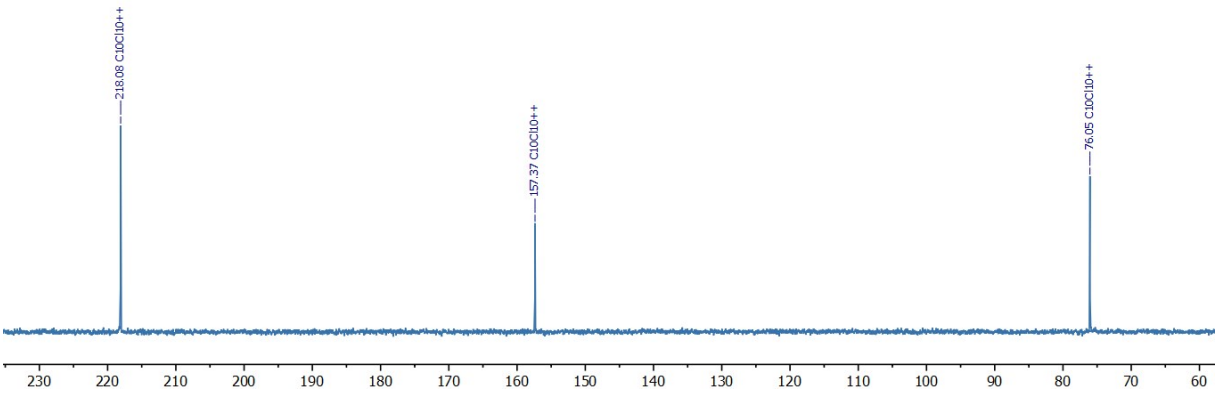

Figure S9: *^{13}C NMR spectrum (100 MHz, SO_2, ext. acetone-d_6, -60 °C).*

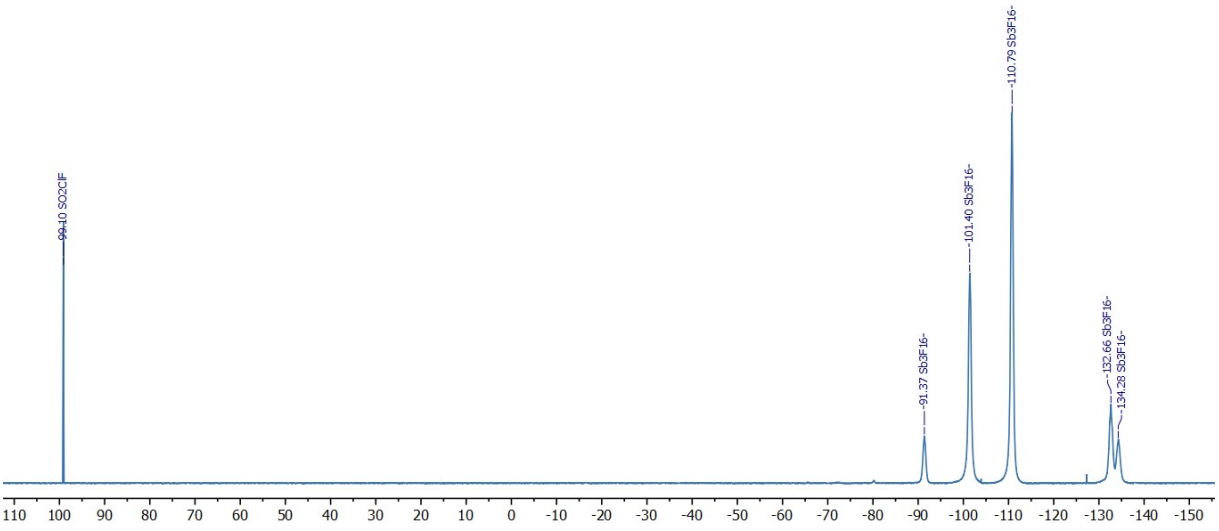

Figure S10: *^{19}F NMR spectrum (377 MHz, SO_2, ext. acetone-d_6, -60 °C).*

C_5Br_6:

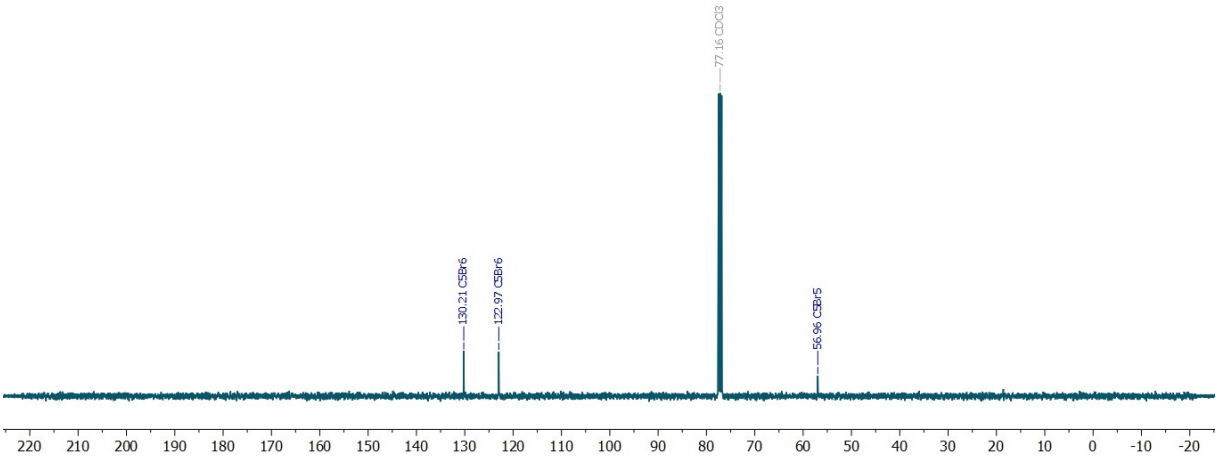

Figure S11: *^{13}C NMR spectrum (100 MHz, $CDCl_3$, r.t.).*

C_5Cl_6:

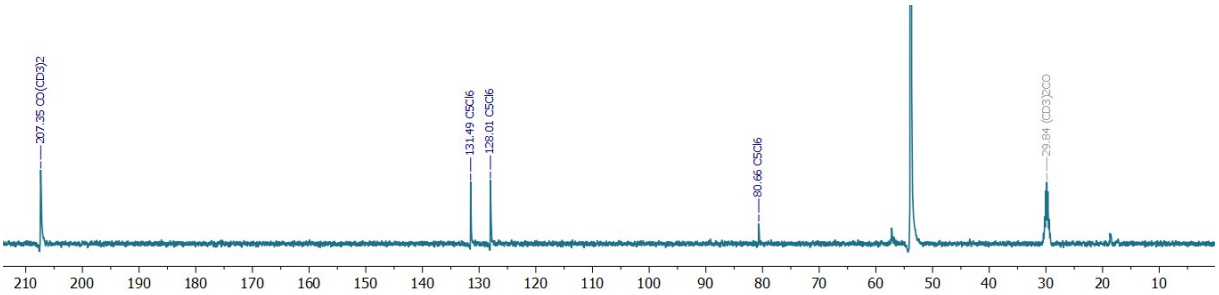

Figure S12: *^{13}C NMR spectrum (100 MHz, CH_2Cl_2, ext. acetone-d_6, r.t.).*

3 Quantum-Chemical Calculations

Structure optimizations and frequency calculations were both performed using B3LYP/Def2TZVP with GD3BJ dispersion correction and MP2/cc-PVTZ with the Gaussian16 (Rev A.03) software.[10] Thermodynamic corrections were taken from these calculations (T = 213.15 K and p = 1 atm). The influence of the solvation was included by calculations using the Polarizable Continuum Model (PCM) using the integral equation formalism variant (IEFPCM). Dielectric constants of ε_r=2; 10 and 23 were used to simulate solvents of different polarity. NBO charges were calculated with NBO Version 3.1.[11] Results were visualized with Chemcraft.[12]

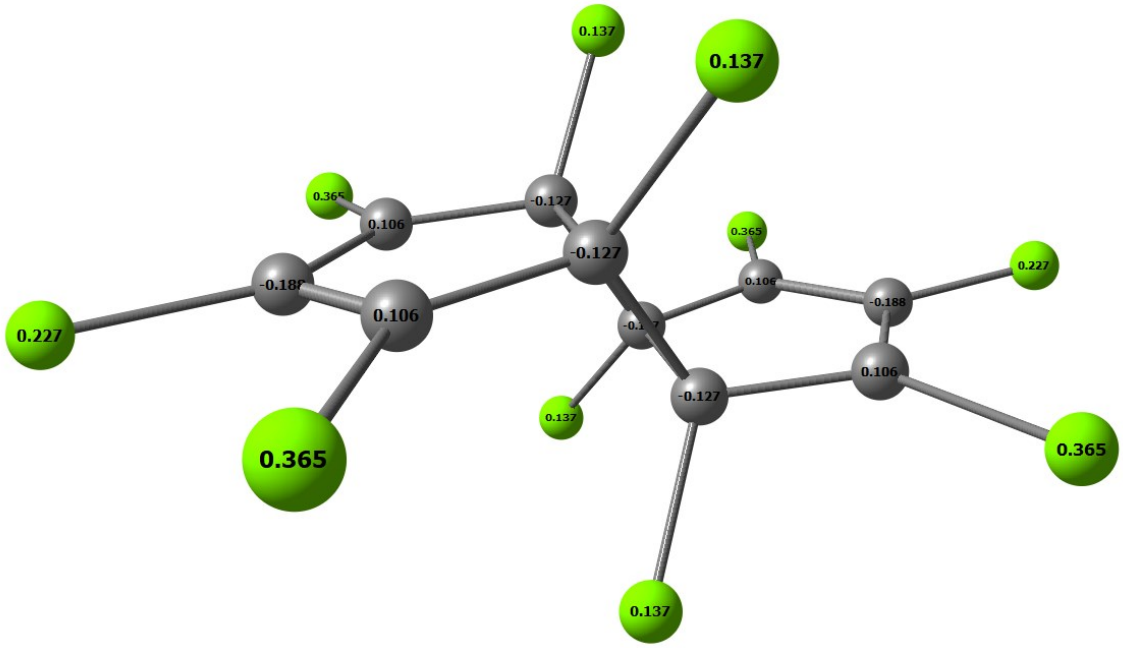

Figure S13: *NBO charges of $C_{10}Cl_{10}^{2+}$ (B3LYP/Def2-TZVP)*

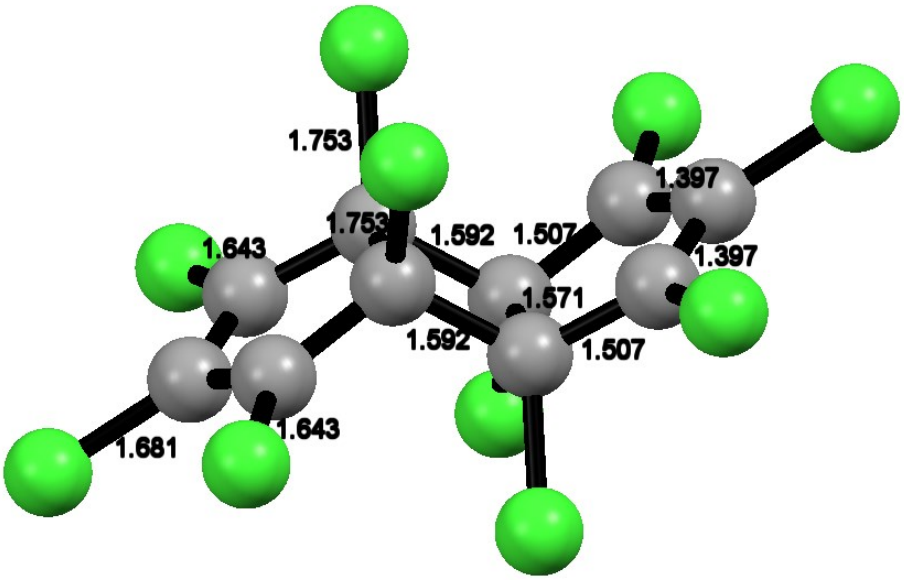

Figure S14: *Optimized Structure of $C_{10}Cl_{10}^{2+}$ (B3LYP/Def2-TZVP) with C-Cl (left) and C-C (right) bond lengths*

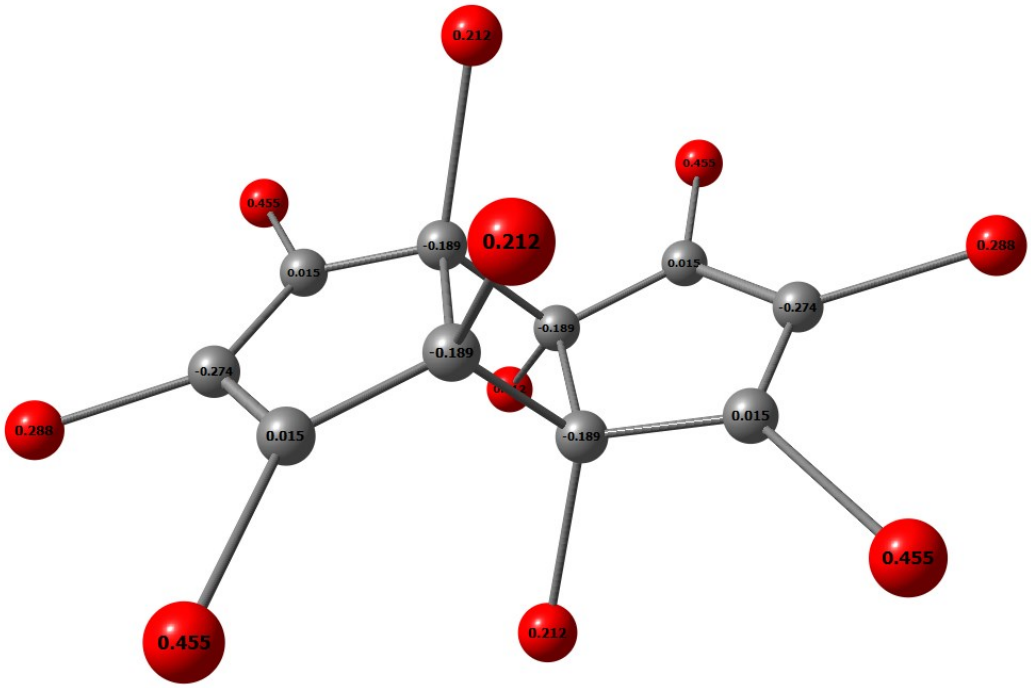

Figure S15: NBO charges of $C_{10}Br_{10}^{2+}$ (B3LYP/Def2-TZVP)

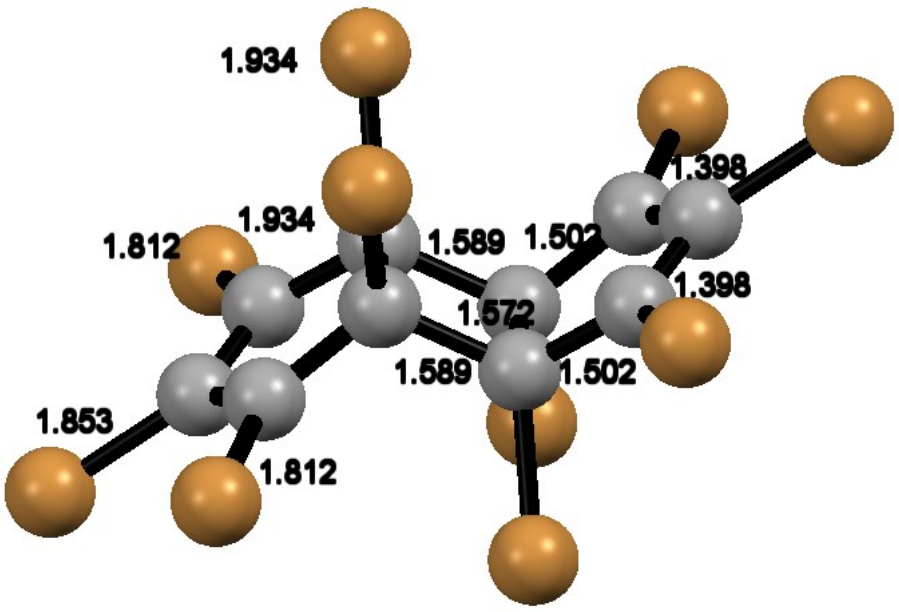

Figure S16: *Optimized Structure of $C_{10}Br_{10}^{2+}$ (B3LYP/Def2-TZVP) with C-Br (left) and C-C (right) bond lengths*

Table S4: *Calculated energy differences ΔG in kJ/mol at 213.15 K. ε_r is the dielectric constant, used for calculations with the polarizable Continuum Model (PCM) for solvent effects*

	B3LYP-GD3BJ/Def2-TZVP	**MP2/cc-PVTZ**
$C_5Cl_5^+$ sing/trip **3a**/**2a**	+ 32 / 0	+15 / 0
2a + **2a** → **4a** / **exo-5a** / **endo-5a**	+225/ + 317 / + 316	+102 / +156 / +165
With ε_r = 2	+108 / +195 /+201	-13 / +37 / +41
With ε_r = 10	+35 / +103 / +101	-109 / -61 / -61
With ε_r = 23	+5 / +89 / +90	-123 / -75 / -76
$C_5Br_5^+$ sing/trip **3b**/**2b**	+31 / 0	
2b + **2b**→ **4b** / **exo-5b** / **endo-5b**	+202 / +296 / +292	
With ε_r = 2	+89 / +185 / +177	
With ε_r = 10	+7 / +97 / +92	
With ε_r = 23	-6 / +81 / +78	

Cartesian coordinates of the optimized structures:

B3LYP-GD3BJ/Def2-TZVP - without solvent:

$C_5Cl_5^+$sing HF=-2491.3896934

Sum of electronic and thermal Free Energies= -2491.379865

17	0.000000000	2.780004000	0.940534000
17	0.000000000	0.000000000	2.798904000
17	0.000000000	-2.780004000	0.940534000
17	0.000000000	-1.675519000	-2.332732000
17	0.000000000	1.675519000	-2.332732000
6	0.000000000	1.199022000	0.343936000
6	0.000000000	0.000000000	1.160088000
6	0.000000000	-1.199022000	0.343936000
6	0.000000000	-0.774627000	-0.944535000
6	0.000000000	0.774627000	-0.944535000

$C_5Cl_5^+$trip HF=-2491.4023133

Sum of electronic and thermal Free Energies= -2491.392079

17	0.000000000	2.736995000	0.889192000
17	0.000000000	0.000000000	2.877852000
17	0.000000000	-2.736995000	0.889192000
17	0.000000000	-1.691740000	-2.328101000
17	0.000000000	1.691740000	-2.328101000
6	0.000000000	1.153176000	0.374730000
6	0.000000000	0.000000000	1.212764000
6	0.000000000	-1.153176000	0.374730000
6	0.000000000	-0.712754000	-0.981161000

6	0.000000000	0.712754000	-0.981161000

$C_{10}Cl_{10}^{2+}$ HF=-4982.7402342

Sum of electronic and thermal Free Energies= -4982.698577

17	2.461574000	-2.686488000	-0.144544000
17	-0.027070000	-1.608036000	-2.071211000
17	-0.027113000	1.607997000	-2.071223000
17	0.027070000	-1.608034000	2.071213000
17	-2.461573000	-2.686488000	0.144543000
17	0.027113000	1.607999000	2.071223000
17	4.353903000	0.000019000	0.293611000
17	2.461557000	2.686504000	-0.144625000
17	-4.353902000	0.000018000	-0.293612000
17	-2.461558000	2.686504000	0.144623000
6	2.718033000	0.000010000	-0.093706000
6	1.926562000	1.137777000	-0.272077000
6	1.926568000	-1.137770000	-0.272039000
6	0.502636000	0.785458000	-0.616968000
6	0.502644000	-0.785467000	-0.616958000
6	-0.502644000	-0.785467000	0.616960000
6	-0.502636000	0.785458000	0.616969000
6	-1.926568000	-1.137770000	0.272040000
6	-2.718033000	0.000009000	0.093706000
6	-1.926562000	1.137777000	0.272077000

$C_{10}Cl_{10}^{2+}$exo HF=-4982.7042718

Sum of electronic and thermal Free Energies= -4982.663353

17	-2.948641000	-0.987564000	0.000000000
17	0.510191000	-3.372823000	1.700929000
17	0.510191000	-3.372823000	-1.700929000
17	-1.043138000	-0.732971000	2.761762000
17	-1.043138000	-0.732971000	-2.761762000
17	2.208442000	0.062291000	-1.564407000
17	2.208442000	0.062291000	1.564407000
17	0.113477000	2.379841000	2.672071000
17	0.113477000	2.379841000	-2.672071000
17	-0.599002000	4.153888000	0.000000000
6	0.178177000	-2.101751000	0.688776000
6	-0.376700000	-0.736567000	1.161009000
6	0.178177000	-2.101751000	-0.688776000
6	-0.376700000	-0.736567000	-1.161009000
6	-1.330957000	-0.793710000	0.000000000
6	0.656829000	0.391060000	0.798815000
6	0.656829000	0.391060000	-0.798815000
6	0.202293000	1.794886000	-1.137440000

6	0.202293000	1.794886000	1.137440000
6	-0.076099000	2.554622000	0.000000000

$C_{10}Cl_{10}^{2+}$endo HF=-4982.7031388

Sum of electronic and thermal Free Energies= -4982.663620

17	-1.651253000	-2.769307000	-0.219095000
17	-1.668275000	2.759177000	-0.228546000
17	0.149069000	-1.540218000	-2.535760000
17	0.144472000	1.536149000	-2.538645000
17	2.026800000	2.691934000	-0.012596000
17	3.823304000	0.010320000	0.743762000
17	2.043116000	-2.682016000	-0.012864000
17	-0.703470000	-1.706815000	2.708727000
17	-0.715942000	1.711997000	2.703461000
17	-3.544688000	-0.011446000	-0.581512000
6	-0.807572000	-0.684236000	1.397977000
6	-0.812317000	0.684616000	1.395879000
6	-1.019626000	-1.166226000	-0.059630000
6	-1.953531000	-0.006054000	-0.295981000
6	-1.026844000	1.160597000	-0.063454000
6	0.239245000	0.795413000	-0.945760000
6	0.243462000	-0.796232000	-0.944383000
6	1.560121000	-1.134088000	-0.297559000
6	1.553366000	1.141106000	-0.297714000
6	2.298151000	0.005743000	0.034324000

B3LYP-GD3BJ/Def2-TZVP with solvent model ε_r=2:

$C_5Cl_5^+$trip HF=-2491.4391029

Sum of electronic and thermal Free Energies= -2491.429110

17	0.000000000	2.737489000	0.883976000
17	0.000000000	0.000000000	2.878598000
17	0.000000000	-2.737489000	0.883976000
17	0.000000000	-1.697106000	-2.323490000
17	0.000000000	1.697106000	-2.323490000
6	0.000000000	1.151950000	0.374520000
6	0.000000000	0.000000000	1.213241000
6	0.000000000	-1.151950000	0.374520000
6	0.000000000	-0.712407000	-0.980530000
6	0.000000000	0.712407000	-0.980530000

$C_{10}Cl_{10}^{2+}$ HF=-4982.8603122
Sum of electronic and thermal Free Energies= -4982.817201

17	-2.459574000	2.684585000	-0.120883000
17	0.018833000	1.622678000	-2.060569000
17	0.019339000	-1.603900000	-2.074259000
17	-0.018446000	1.603213000	2.076714000
17	2.452935000	2.686004000	0.133221000
17	-0.018677000	-1.622143000	2.064020000
17	-4.357835000	-0.004455000	0.273795000
17	-2.454087000	-2.685606000	-0.132524000
17	4.353825000	0.004679000	-0.291835000
17	2.463609000	-2.684636000	0.132347000
6	-2.718132000	-0.001929000	-0.098125000
6	-1.924110000	-1.137484000	-0.268875000
6	-1.928411000	1.136933000	-0.263454000
6	-0.502588000	-0.783260000	-0.616790000
6	-0.504816000	0.787543000	-0.611002000
6	0.503204000	0.782836000	0.619272000
6	0.505496000	-0.788078000	0.614215000
6	1.923726000	1.137422000	0.267552000
6	2.716728000	0.001977000	0.091585000
6	1.929119000	-1.137145000	0.265546000

$C_{10}Cl_{10}^{2+}$exo HF=-4982.8254363
Sum of electronic and thermal Free Energies= -4982.783801

17	-0.922502000	0.041147000	2.954650000
17	-3.354175000	-1.749209000	-0.459223000
17	-3.383359000	1.671715000	-0.550033000
17	-0.699567000	-2.741035000	1.098906000
17	-0.765308000	2.780587000	0.994096000
17	0.088546000	1.567051000	-2.212384000
17	0.010055000	-1.554747000	-2.201971000
17	2.365218000	-2.675303000	-0.152576000
17	2.352344000	2.670295000	-0.045807000
17	4.160744000	-0.009054000	0.543364000
6	-2.103020000	-0.704970000	-0.147688000
6	-0.728106000	-1.153066000	0.401681000
6	-2.114236000	0.669378000	-0.179994000
6	-0.751267000	1.166486000	0.362914000
6	-0.774069000	0.021349000	1.336347000
6	0.380224000	-0.795654000	-0.656758000
6	0.383479000	0.800591000	-0.656309000
6	1.784138000	1.134514000	-0.189390000
6	1.789346000	-1.138253000	-0.228437000
6	2.552857000	-0.004473000	0.045408000

$C_{10}Cl_{10}^{2+}$endo HF=-4982.8251481
Sum of electronic and thermal Free Energies= -4982.781793

17	1.646315000	2.764467000	-0.237956000
17	1.644853000	-2.765247000	-0.238454000
17	-0.149192000	1.530836000	-2.553798000
17	-0.151245000	-1.529321000	-2.554596000
17	-2.053914000	-2.685642000	-0.065560000
17	-3.759812000	0.000437000	0.873437000
17	-2.053039000	2.686592000	-0.064721000
17	0.721732000	1.708785000	2.696833000
17	0.720648000	-1.709567000	2.696654000
17	3.546219000	-0.001345000	-0.516634000
6	0.800826000	0.684489000	1.386439000
6	0.800108000	-0.685237000	1.386275000
6	1.012635000	1.163124000	-0.070830000
6	1.947724000	-0.000580000	-0.283751000
6	1.011856000	-1.163660000	-0.071118000
6	-0.249142000	-0.793811000	-0.960637000
6	-0.248668000	0.794395000	-0.960348000
6	-1.559759000	1.136959000	-0.303382000
6	-1.560025000	-1.136108000	-0.303268000
6	-2.274487000	0.000444000	0.080873000

B3LYP-GD3BJ/Def2-TZVP with solvent model ε_r=10:

$C_5Cl_5^{+}$trip HF=-2491.4687201
Sum of electronic and thermal Free Energies= -2491.458731

17	0.000000000	2.735835000	0.886897000
17	0.000000000	0.000000000	2.876846000
17	0.000000000	-2.735835000	0.886897000
17	0.000000000	-1.693209000	-2.325297000
17	0.000000000	1.693209000	-2.325297000
6	0.000000000	1.151334000	0.374077000
6	0.000000000	0.000000000	1.211487000
6	0.000000000	-1.151334000	0.374077000
6	0.000000000	-0.711818000	-0.979887000
6	0.000000000	0.711818000	-0.979887000

$C_{10}Cl_{10}^{2+}$ HF=-4982.9533426
Sum of electronic and thermal Free Energies= -4982.910637

17	-2.452953000	-2.684127000	0.126175000
17	0.024791000	-1.613929000	2.066566000
17	0.024928000	1.607087000	2.070733000
17	-0.025226000	-1.606858000	-2.070819000
17	2.449036000	-2.684629000	-0.129147000
17	-0.024651000	1.614144000	-2.066464000

17	-4.353426000	0.002270000	-0.276411000
17	-2.448970000	2.684535000	0.128020000
17	4.353416000	-0.002561000	0.276516000
17	2.452947000	2.684085000	-0.125063000
6	-2.713964000	0.000776000	0.102421000
6	-1.922809000	1.136615000	0.270234000
6	-1.925118000	-1.136647000	0.269886000
6	-0.501670000	0.784022000	0.617505000
6	-0.502464000	-0.785693000	0.615823000
6	0.501658000	-0.783923000	-0.617567000
6	0.502592000	0.785728000	-0.615777000
6	1.922833000	-1.136667000	-0.270674000
6	2.714045000	-0.000862000	-0.102459000
6	1.925205000	1.136604000	-0.269689000

$C_{10}Cl_{10}^{2+}$exo HF=-4982.9204234

Sum of electronic and thermal Free Energies= -4982.878125

17	-0.893371000	0.000004000	2.953932000
17	-3.375758000	-1.701694000	-0.493888000
17	-3.375761000	1.701687000	-0.493900000
17	-0.735525000	-2.764793000	1.040475000
17	-0.735531000	2.764796000	1.040466000
17	0.041360000	1.560525000	-2.207533000
17	0.041352000	-1.560523000	-2.207532000
17	2.359834000	-2.671181000	-0.099351000
17	2.359835000	2.671179000	-0.099339000
17	4.159397000	-0.000002000	0.534267000
6	-2.106453000	-0.685039000	-0.157892000
6	-0.738508000	-1.159879000	0.383973000
6	-2.106454000	0.685037000	-0.157896000
6	-0.738510000	1.159881000	0.383970000
6	-0.759721000	0.000002000	1.341318000
6	0.381170000	-0.798312000	-0.657273000
6	0.381171000	0.798313000	-0.657273000
6	1.786810000	1.136335000	-0.212612000
6	1.786810000	-1.136335000	-0.212617000
6	2.550498000	-0.000001000	0.038113000

$C_{10}Cl_{10}^{2+}$endo HF=-4982.9200142
Sum of electronic and thermal Free Energies= -4982.878870

17	-1.610171000	-2.780186000	-0.278008000
17	-1.670514000	2.744024000	-0.280071000
17	0.251429000	-1.533159000	-2.531698000
17	0.211200000	1.538926000	-2.530429000
17	2.026410000	2.707196000	0.024700000
17	3.800297000	0.042342000	0.871492000

17	2.087878000	-2.661065000	0.023542000
17	-0.816375000	-1.709891000	2.690633000
17	-0.886239000	1.691127000	2.690869000
17	-3.515337000	-0.040542000	-0.664884000
6	-0.847471000	-0.693561000	1.372876000
6	-0.870381000	0.674461000	1.373278000
6	-0.995645000	-1.173458000	-0.089965000
6	-1.935509000	-0.021862000	-0.344617000
6	-1.023896000	1.150726000	-0.090320000
6	0.270490000	0.797706000	-0.934167000
6	0.289110000	-0.791846000	-0.934763000
6	1.591100000	-1.119119000	-0.252960000
6	1.564892000	1.154526000	-0.252646000
6	2.301339000	0.025903000	0.107536000

B3LYP-GD3BJ/Def2-TZVP with solvent model ε_r=23:

$C_5Cl_5^+$trip HF=-2491.4730825

Sum of electronic and thermal Free Energies= -2491.463044

17	0.000000000	2.735724000	0.887247000
17	0.000000000	0.000000000	2.876693000
17	0.000000000	-2.735724000	0.887247000
17	0.000000000	-1.692158000	-2.325646000
17	0.000000000	1.692158000	-2.325646000
6	0.000000000	1.151263000	0.374130000
6	0.000000000	0.000000000	1.211265000
6	0.000000000	-1.151263000	0.374130000
6	0.000000000	-0.711682000	-0.979613000
6	0.000000000	0.711682000	-0.979613000

$C_{10}Cl_{10}^{2+}$ HF=-4982.967049

Sum of electronic and thermal Free Energies= -4982.924052

17	-2.450970000	-2.684756000	0.127777000
17	0.029038000	-1.611820000	2.066897000
17	0.025352000	1.608078000	2.070507000
17	-0.025546000	-1.607956000	-2.070512000
17	2.448971000	-2.683688000	-0.128722000
17	-0.029036000	1.611913000	-2.066745000
17	-4.352438000	0.000836000	-0.276004000
17	-2.448867000	2.683656000	0.128077000
17	4.352497000	-0.000992000	0.275773000

17	2.450906000	2.684757000	-0.126993000
6	-2.712981000	-0.000184000	0.104083000
6	-1.922644000	1.135861000	0.271097000
6	-1.923963000	-1.137105000	0.271913000
6	-0.501408000	0.783985000	0.617962000
6	-0.501341000	-0.785554000	0.616593000
6	0.501406000	-0.783938000	-0.617925000
6	0.501427000	0.785524000	-0.616482000
6	1.922685000	-1.135893000	-0.271418000
6	2.713079000	0.000151000	-0.104228000
6	1.924003000	1.137075000	-0.271749000

$C_{10}Cl_{10}^{2+}$exo HF=-4982.9346319

Sum of electronic and thermal Free Energies= -4982.892349

17	-0.886014000	0.000000000	2.955235000
17	-3.376213000	-1.700969000	-0.490497000
17	-3.376214000	1.700966000	-0.490498000
17	-0.732055000	-2.765037000	1.040357000
17	-0.732058000	2.765037000	1.040357000
17	0.036268000	1.561900000	-2.207619000
17	0.036268000	-1.561899000	-2.207619000
17	2.358478000	-2.671203000	-0.103213000
17	2.358476000	2.671205000	-0.103212000
17	4.157694000	0.000001000	0.534667000
6	-2.105809000	-0.684614000	-0.154866000
6	-0.737563000	-1.159531000	0.385398000
6	-2.105809000	0.684614000	-0.154866000
6	-0.737564000	1.159531000	0.385398000
6	-0.756185000	0.000000000	1.343793000
6	0.380242000	-0.798202000	-0.658466000
6	0.380242000	0.798202000	-0.658466000
6	1.786664000	1.136135000	-0.216758000
6	1.786664000	-1.136135000	-0.216759000
6	2.549334000	0.000001000	0.036380000

$C_{10}Cl_{10}^{2+}$endo HF=-4982.9338988
Sum of electronic and thermal Free Energies= -4982.891798

17	-1.638303000	-2.762973000	-0.283690000
17	-1.641512000	2.761019000	-0.285257000
17	0.242215000	-1.537422000	-2.528929000
17	0.241321000	1.537007000	-2.529306000
17	2.055068000	2.684646000	0.035444000
17	3.803434000	0.001995000	0.874120000
17	2.058220000	-2.682647000	0.035292000

17	-0.865127000	-1.699757000	2.688660000
17	-0.867932000	1.700289000	2.687781000
17	-3.512107000	-0.002196000	-0.677590000
6	-0.862885000	-0.684052000	1.370414000
6	-0.863892000	0.683894000	1.370068000
6	-1.008114000	-1.162510000	-0.093163000
6	-1.933679000	-0.001170000	-0.351347000
6	-1.009491000	1.161393000	-0.093796000
6	0.283289000	0.794882000	-0.932738000
6	0.284124000	-0.794915000	-0.932557000
6	1.580638000	-1.135946000	-0.247274000
6	1.579324000	1.137393000	-0.247236000
6	2.304066000	0.001141000	0.110808000

B3LYP-GD3BJ/Def2-TZVP without solvent model:

$C_5Br_5^+$sing HF=-13061.1724738

Sum of electronic and thermal Free Energies= -13061.170006

35	-3.100449000	-0.028385000	0.000000000
35	-0.918052000	-2.825187000	0.000000000
35	2.491126000	-1.845519000	0.000000000
35	2.453969000	1.787336000	0.000000000
35	-0.934792000	2.887120000	0.000000000
6	-1.244274000	0.038856000	0.000000000
6	-0.360969000	-1.109386000	0.000000000
6	1.030035000	-0.699173000	0.000000000
6	1.025604000	0.658952000	0.000000000
6	-0.441748000	1.135388000	0.000000000

$C_5Br_5^+$trip HF=-13061.1846056

Sum of electronic and thermal Free Energies= -13061.181684

35	-3.043417000	0.000006000	0.000000000
35	-0.940604000	-2.894661000	0.000000000
35	2.462291000	-1.789061000	0.000000000
35	2.462317000	1.789031000	0.000000000
35	-0.940552000	2.894682000	0.000000000
6	-1.212321000	0.000017000	0.000000000
6	-0.374568000	-1.153102000	0.000000000
6	0.980925000	-0.712695000	0.000000000
6	0.980932000	0.712684000	0.000000000
6	-0.374556000	1.153104000	0.000000000

$C_{10}Br_{10}^{2+}$ HF=-26122.3146486
Sum of electronic and thermal Free Energies= -26122.286541

35	-2.841237000	-4.381696000	-0.083774000
35	0.440877000	-3.339976000	-0.731297000
35	-6.855612000	-1.279170000	0.053696000
35	-6.662813000	2.181100000	0.569869000
35	-4.002665000	-1.963610000	2.178057000
35	0.633674000	0.120328000	-0.215366000
35	-1.935053000	0.715075000	2.099833000
35	-4.286802000	-1.873891000	-2.261405000
35	-2.219296000	0.804870000	-2.339607000
35	-3.380730000	3.222884000	-0.077700000
6	-2.261559000	-2.671045000	0.064005000
6	-0.953913000	-2.247511000	-0.189432000
6	-0.869087000	-0.866898000	0.011218000
6	-3.139979000	-1.533213000	0.501082000
6	-2.179685000	-0.289104000	0.464727000
6	-3.081952000	0.374417000	-0.662635000
6	-4.042239000	-0.869702000	-0.626302000
6	-3.960385000	1.512227000	-0.225512000
6	-5.352845000	-0.291931000	-0.172792000
6	-5.268023000	1.088672000	0.027927000

$C_{10}Br_{10}^{2+}$exo HF=-26122.2779017
Sum of electronic and thermal Free Energies= -26122.250623

35	4.336546000	-0.000999000	0.653870000
35	2.493339000	2.820862000	-0.117830000
35	2.493087000	-2.821349000	-0.123140000
35	0.050072000	-1.663250000	-2.342653000
35	0.053939000	1.664268000	-2.342806000
35	-0.748197000	2.914880000	1.137070000
35	-0.745516000	-2.913898000	1.139224000
35	-3.497977000	1.779119000	-0.575993000
35	-3.498029000	-1.780891000	-0.571417000
35	-1.042077000	0.001167000	3.111890000
6	2.571804000	-0.000405000	0.081671000
6	1.815359000	-1.139961000	-0.196747000
6	1.815445000	1.139670000	-0.194817000
6	0.411945000	0.801443000	-0.636473000
6	0.411672000	-0.800964000	-0.636833000
6	-0.800994000	0.000527000	1.332053000
6	-0.729334000	1.161577000	0.380628000
6	-2.084565000	0.688035000	-0.183196000
6	-0.728722000	-1.161122000	0.381717000
6	-2.084486000	-0.688710000	-0.181844000

$C_{10}Br_{10}^{2+}$endo HF=-26122.2791026
Sum of electronic and thermal Free Energies= -26122.252298

35	-3.676287000	-0.075590000	-0.748656000
35	-0.948296000	1.915308000	2.746997000
35	-0.601364000	-1.652560000	2.865973000
35	2.144688000	-2.897399000	-0.167488000
35	3.945687000	-0.110075000	0.959216000
35	2.023031000	2.764312000	0.380954000
35	0.479305000	1.670051000	-2.641957000
35	0.083932000	-1.579591000	-2.721791000
35	-1.791274000	2.899926000	-0.464160000
35	-1.669163000	-2.929808000	-0.161065000
6	2.295126000	-0.064372000	0.116917000
6	1.549916000	1.090353000	-0.140477000
6	1.586716000	-1.179760000	-0.339612000
6	0.275929000	-0.796372000	-0.954371000
6	0.295635000	0.794211000	-0.914316000
6	-1.044543000	1.172549000	-0.163244000
6	-1.933856000	-0.018730000	-0.377790000
6	-0.986530000	-1.149277000	-0.060635000
6	-0.900463000	0.755738000	1.325948000
6	-0.806881000	-0.609262000	1.372056000

B3LYP-GD3BJ/Def2-TZVP with solvent model ε_r=2:

$C_5Br_5^{+}$trip HF=-13061.2192113

Sum of electronic and thermal Free Energies= -13061.215658

35	-3.042226000	0.000003000	0.000000000
35	-0.940436000	-2.892942000	0.000000000
35	2.461440000	-1.787838000	0.000000000
35	2.461465000	1.787809000	0.000000000
35	-0.940381000	2.892965000	0.000000000
6	-1.211709000	0.000016000	0.000000000
6	-0.374269000	-1.152245000	0.000000000
6	0.980407000	-0.712267000	0.000000000
6	0.980413000	0.712256000	0.000000000
6	-0.374257000	1.152247000	0.000000000

$C_{10}Br_{10}^{2+}$ HF=-26122.4280355
Sum of electronic and thermal Free Energies= -26122.397526

35	-2.839336000	-4.376420000	-0.059313000
35	0.415617000	-3.323251000	-0.797890000
35	-6.863586000	-1.274994000	0.000505000
35	-6.637787000	2.164470000	0.635757000
35	-4.017836000	-1.941598000	2.180312000

35	0.641643000	0.116110000	-0.162413000
35	-1.946724000	0.744455000	2.086916000
35	-4.274858000	-1.903220000	-2.248375000
35	-2.204165000	0.782867000	-2.341660000
35	-3.382708000	3.217625000	-0.102132000
6	-2.264964000	-2.664812000	0.070361000
6	-0.964355000	-2.237913000	-0.204597000
6	-0.870069000	-0.863314000	0.021765000
6	-3.142819000	-1.527075000	0.509223000
6	-2.181918000	-0.283958000	0.468488000
6	-3.079073000	0.368264000	-0.670499000
6	-4.039916000	-0.874863000	-0.629836000
6	-3.956966000	1.505959000	-0.231664000
6	-5.351842000	-0.295562000	-0.183314000
6	-5.257664000	1.079056000	0.042958000

$C_{10}Br_{10}^{2+}$exo HF=-26122.3918002
Sum of electronic and thermal Free Energies= -26122.360983

35	4.313694000	-0.006181000	0.695121000
35	2.491191000	2.817870000	-0.107989000
35	2.487508000	-2.819760000	-0.146571000
35	0.020092000	-1.646158000	-2.347191000
35	0.076753000	1.658868000	-2.350824000
35	-0.752952000	2.913693000	1.132671000
35	-0.729050000	-2.909098000	1.143577000
35	-3.499057000	1.768142000	-0.600803000
35	-3.498723000	-1.785806000	-0.555419000
35	-0.998540000	0.004284000	3.110168000
6	2.564319000	-0.002285000	0.083229000
6	1.810673000	-1.139465000	-0.204398000
6	1.810835000	1.139322000	-0.186863000
6	0.410807000	0.803517000	-0.638452000
6	0.407336000	-0.797487000	-0.642164000
6	-0.790651000	0.003063000	1.329917000
6	-0.732856000	1.162587000	0.375086000
6	-2.086347000	0.684249000	-0.185522000
6	-0.726271000	-1.158941000	0.383382000
6	-2.085452000	-0.690416000	-0.172579000

$C_{10}Br_{10}^{2+}$endo HF=-26122.3939956
Sum of electronic and thermal Free Energies= -26122.363923

35	-3.674687000	-0.013084000	-0.757517000
35	-0.772522000	1.829288000	2.786625000
35	-0.696072000	-1.745795000	2.825028000
35	2.113691000	-2.861792000	0.004887000
35	3.902664000	-0.035300000	1.027203000
35	2.070758000	2.818430000	0.179936000

35	0.321157000	1.645377000	-2.682983000
35	0.220059000	-1.620382000	-2.707737000
35	-1.752572000	2.914136000	-0.348038000
35	-1.718505000	-2.922961000	-0.266483000
6	2.278404000	-0.022137000	0.135411000
6	1.561115000	1.123775000	-0.214573000
6	1.570753000	-1.154635000	-0.272569000
6	0.279592000	-0.798180000	-0.948113000
6	0.285745000	0.795480000	-0.935961000
6	-1.024993000	1.165070000	-0.126493000
6	-1.937242000	-0.003819000	-0.380076000
6	-1.011746000	-1.158017000	-0.099088000
6	-0.858913000	0.705198000	1.339885000
6	-0.835377000	-0.661005000	1.353154000

B3LYP-GD3BJ/Def2-TZVP with solvent model ε_r=10

$C_5Br_5^+$trip HF=-13061.2470708

Sum of electronic and thermal Free Energies= -13061.244543

35	-3.041161000	0.000004000	0.000000000
35	-0.940051000	-2.892531000	0.000000000
35	2.460618000	-1.787698000	0.000000000
35	2.460645000	1.787668000	0.000000000
35	-0.939998000	2.892553000	0.000000000
6	-1.210820000	0.000017000	0.000000000
6	-0.374094000	-1.151607000	0.000000000
6	0.979693000	-0.711818000	0.000000000
6	0.979700000	0.711807000	0.000000000
6	-0.374083000	1.151609000	0.000000000

$C_{10}Br_{10}^{2+}$ HF=-26122.5152669
Sum of electronic and thermal Free Energies= -26122.486282

35	-2.851036000	-4.370830000	-0.087987000
35	0.429238000	-3.333652000	-0.745619000
35	-6.846410000	-1.286988000	0.047931000
35	-6.651296000	2.174676000	0.584063000
35	-4.010449000	-1.955780000	2.176695000
35	0.624502000	0.128053000	-0.209806000
35	-1.939651000	0.726897000	2.092881000
35	-4.282048000	-1.885717000	-2.254482000
35	-2.211516000	0.797255000	-2.338167000
35	-3.370999000	3.212015000	-0.073222000
6	-2.264687000	-2.666401000	0.066610000
6	-0.960454000	-2.241459000	-0.188011000
6	-0.871962000	-0.864469000	0.015431000
6	-3.142046000	-1.529812000	0.504627000

6	-2.181897000	-0.287386000	0.466975000
6	-3.079878000	0.371071000	-0.666130000
6	-4.039966000	-0.871409000	-0.628558000
6	-3.957280000	1.507578000	-0.227992000
6	-5.349964000	-0.294395000	-0.177116000
6	-5.261526000	1.082577000	0.026469000

$C_{10}Br_{10}^{2+}$exo HF=-26122.4805635
Sum of electronic and thermal Free Energies= -26122.452311

35	4.312610000	-0.011205000	0.688321000
35	2.480730000	2.815804000	-0.085310000
35	2.477805000	-2.822530000	-0.151740000
35	0.015368000	-1.649144000	-2.343915000
35	0.069390000	1.666469000	-2.344287000
35	-0.764652000	2.918606000	1.122397000
35	-0.732592000	-2.905965000	1.148325000
35	-3.493477000	1.767505000	-0.616295000
35	-3.490171000	-1.792959000	-0.565466000
35	-0.967688000	0.012762000	3.110378000
6	2.558644000	-0.005386000	0.084690000
6	1.808118000	-1.141210000	-0.206755000
6	1.808506000	1.136959000	-0.182029000
6	0.409780000	0.803911000	-0.636913000
6	0.405771000	-0.797518000	-0.641471000
6	-0.775847000	0.007192000	1.335706000
6	-0.734701000	1.162745000	0.375821000
6	-2.085023000	0.680249000	-0.190246000
6	-0.726276000	-1.156222000	0.388070000
6	-2.082987000	-0.690065000	-0.174908000

$C_{10}Br_{10}^{2+}$endo HF=-26122.4823529
Sum of electronic and thermal Free Energies= -26122.453957

35	-3.674718000	-0.003484000	-0.737798000
35	-0.771234000	1.807970000	2.795219000
35	-0.725358000	-1.774307000	2.808394000
35	2.074673000	-2.850320000	0.085489000
35	3.925662000	-0.019456000	0.984751000
35	2.060204000	2.828090000	0.163322000
35	0.312461000	1.640207000	-2.688770000
35	0.253824000	-1.629307000	-2.700439000
35	-1.735805000	2.916825000	-0.333027000
35	-1.728581000	-2.915727000	-0.295278000
6	2.289333000	-0.011090000	0.115173000
6	1.564928000	1.130565000	-0.228825000
6	1.568444000	-1.145818000	-0.257928000
6	0.281629000	-0.796070000	-0.944980000

6	0.285840000	0.795319000	-0.938532000
6	-1.018718000	1.162991000	-0.120951000
6	-1.937430000	0.000640000	-0.374371000
6	-1.013911000	-1.157242000	-0.108313000
6	-0.851105000	0.692841000	1.342126000
6	-0.838829000	-0.672977000	1.347235000

B3LYP-GD3BJ/Def2-TZVP with solvent model ε_r=23

$C_5Br_5^+$trip HF=-13061.2511821
Sum of electronic and thermal Free Energies= -13061.248536

35	-3.040986000	0.000004000	0.000000000
35	-0.939779000	-2.892442000	0.000000000
35	2.460254000	-1.787717000	0.000000000
35	2.460281000	1.787687000	0.000000000
35	-0.939727000	2.892465000	0.000000000
6	-1.210633000	0.000017000	0.000000000
6	-0.374024000	-1.151477000	0.000000000
6	0.979533000	-0.711709000	0.000000000
6	0.979540000	0.711697000	0.000000000
6	-0.374013000	1.151479000	0.000000000

$C_{10}Br_{10}^{2+}$ HF=-26122.5279817
Sum of electronic and thermal Free Energies= -26122.499512

35	-2.852723000	-4.370673000	-0.096715000
35	0.435573000	-3.336899000	-0.727453000
35	-6.843181000	-1.287680000	0.062542000
35	-6.657479000	2.178024000	0.566098000
35	-4.006215000	-1.961652000	2.175921000
35	0.621235000	0.128855000	-0.224191000
35	-1.936273000	0.720618000	2.095122000
35	-4.285623000	-1.879402000	-2.256739000
35	-2.215755000	0.802880000	-2.337506000
35	-3.369194000	3.211834000	-0.064674000
6	-2.263946000	-2.667659000	0.064915000
6	-0.958451000	-2.243439000	-0.182822000
6	-0.872169000	-0.865313000	0.012932000
6	-3.141205000	-1.531231000	0.502649000
6	-2.181448000	-0.288715000	0.466039000
6	-3.080738000	0.372433000	-0.664234000
6	-4.040487000	-0.870093000	-0.627643000
6	-3.957995000	1.508841000	-0.226440000
6	-5.349772000	-0.293507000	-0.174529000
6	-5.263479000	1.084605000	0.021321000

$C_{10}Br_{10}^{2+}$exo HF=-26122.4939119
Sum of electronic and thermal Free Energies= -26122.466199

35	4.313705000	-0.011119000	0.683645000
35	2.477988000	2.815814000	-0.082426000
35	2.475837000	-2.822694000	-0.146562000
35	0.018130000	-1.652172000	-2.342418000
35	0.063047000	1.668535000	-2.341563000
35	-0.766799000	2.919725000	1.120515000
35	-0.737196000	-2.907044000	1.147090000
35	-3.491704000	1.769483000	-0.620536000
35	-3.488871000	-1.792829000	-0.574486000
35	-0.953102000	0.013001000	3.111946000
6	2.557991000	-0.005309000	0.085137000
6	1.807533000	-1.141071000	-0.205389000
6	1.808057000	1.136532000	-0.182486000
6	0.408887000	0.803548000	-0.636069000
6	0.405316000	-0.797996000	-0.640269000
6	-0.772628000	0.006832000	1.338339000
6	-0.735575000	1.162016000	0.377640000
6	-2.085527000	0.679960000	-0.190411000
6	-0.728014000	-1.156066000	0.389059000
6	-2.083766000	-0.689150000	-0.176382000

$C_{10}Br_{10}^{2+}$endo HF=-26122.4953277
Sum of electronic and thermal Free Energies= -26122.467367

35	-3.676733000	0.000445000	-0.729313000
35	-0.765473000	1.799482000	2.798327000
35	-0.742915000	-1.782967000	2.803798000
35	2.066224000	-2.846219000	0.108181000
35	3.931335000	-0.012397000	0.973872000
35	2.062036000	2.831875000	0.150442000
35	0.305233000	1.638819000	-2.691040000
35	0.271560000	-1.632302000	-2.698176000
35	-1.730945000	2.917948000	-0.324725000
35	-1.731582000	-2.914627000	-0.306199000
6	2.291420000	-0.007207000	0.111508000
6	1.566448000	1.133022000	-0.234791000
6	1.566913000	-1.142837000	-0.250618000
6	0.282358000	-0.795623000	-0.943589000
6	0.285579000	0.795311000	-0.939752000
6	-1.016666000	1.162083000	-0.118359000
6	-1.938331000	0.001761000	-0.372416000
6	-1.015648000	-1.157597000	-0.112371000
6	-0.847561000	0.688295000	1.342740000
6	-0.841942000	-0.677614000	1.344976000

MP2/cc-PVTZ (without solvent):

$C_5Cl_5^+$sing MP2=-2488.3011085

Sum of electronic and thermal Free Energies= -2488.291834

17	0.863060000	-2.674229000	0.000000000
17	2.937720000	-0.000951000	0.000000000
17	0.863060000	2.676225000	0.000000000
17	-2.325886000	1.749475000	0.000000000
17	-2.326387000	-1.750865000	0.000000000
6	0.401383000	-1.105716000	0.000000000
6	1.254259000	0.000849000	0.000000000
6	0.403188000	1.106792000	0.000000000
6	-1.045803000	0.674834000	0.000000000
6	-1.045803000	-0.675782000	0.000000000

$C_5Cl_5^+$trip MP2=-2488.3099986
Sum of electronic and thermal Free Energies= -2488.297552

17	-0.887538000	2.731587000	0.000000000
17	-2.872164000	0.000000000	0.000000000
17	-0.887538000	-2.731587000	0.000000000
17	2.323620000	-1.688228000	0.000000000
17	2.323620000	1.688228000	0.000000000
6	-0.375315000	1.155097000	0.000000000
6	-1.214560000	0.000000000	0.000000000
6	-0.375315000	-1.155098000	0.000000000
6	0.982597000	-0.713895000	0.000000000
6	0.982596000	0.713895000	0.000000000

$C_{10}Cl_{10}^{2+}$ MP2=-4976.5986755
Sum of electronic and thermal Free Energies= -4976.556388

17	-2.435550000	-2.680403000	0.189064000
17	0.076448000	-1.604146000	2.061405000
17	0.076554000	1.604055000	2.061422000
17	-0.076447000	-1.604145000	-2.061405000
17	2.435550000	-2.680403000	-0.189065000
17	-0.076555000	1.604057000	-2.061421000
17	-4.318201000	0.000047000	-0.304019000
17	-2.435499000	2.680441000	0.189244000
17	4.318201000	0.000049000	0.304019000
17	2.435499000	2.680441000	-0.189243000
6	-2.697648000	0.000023000	0.098382000
6	-1.900000000	1.135304000	0.296590000
6	-1.900020000	-1.135286000	0.296518000
6	-0.482547000	0.782558000	0.632470000
6	-0.482564000	-0.782588000	0.632450000
6	0.482563000	-0.782588000	-0.632450000

6	0.482547000	0.782558000	-0.632470000
6	1.900020000	-1.135286000	-0.296519000
6	2.697648000	0.000023000	-0.098383000
6	1.899999000	1.135303000	-0.296589000

$C_{10}Cl_{10}^{2+}$exo MP2=-4976.5772402
Sum of electronic and thermal Free Energies= -4976.535729

17	-2.836111000	-1.278728000	0.000000000
17	0.477407000	-3.365475000	1.676175000
17	0.477407000	-3.365475000	-1.676175000
17	-0.977377000	-0.719785000	2.755992000
17	-0.977377000	-0.719785000	-2.755992000
17	2.223439000	0.156444000	-1.557152000
17	2.223439000	0.156444000	1.557152000
17	0.078454000	2.401447000	2.661059000
17	0.078454000	2.401447000	-2.661059000
17	-0.806291000	4.108349000	0.000000000
6	0.249900000	-2.049890000	0.701083000
6	-0.309789000	-0.707487000	1.167826000
6	0.249900000	-2.049890000	-0.701083000
6	-0.309789000	-0.707487000	-1.167826000
6	-1.239558000	-0.896729000	0.000000000
6	0.674342000	0.436379000	0.791812000
6	0.674342000	0.436379000	-0.791812000
6	0.154920000	1.810575000	-1.133911000
6	0.154920000	1.810575000	1.133911000
6	-0.189947000	2.555405000	0.000000000

$C_{10}Cl_{10}^{2+}$endo MP2=-4976.5747062
Sum of electronic and thermal Free Energies= -4976.532167

17	1.562659000	2.764995000	-0.406092000
17	1.589780000	-2.748949000	-0.418246000
17	-0.418185000	1.533719000	-2.541185000
17	-0.409562000	-1.531773000	-2.543983000
17	-2.017957000	-2.690204000	0.146024000
17	-3.697809000	-0.016710000	1.157959000
17	-2.045479000	2.673162000	0.144444000
17	1.071326000	1.681762000	2.588727000
17	1.090372000	-1.683013000	2.581646000
17	3.492109000	0.017890000	-0.621293000
6	0.888056000	0.699177000	1.263570000
6	0.895719000	-0.696942000	1.260702000
6	0.944928000	1.175304000	-0.189048000
6	1.881470000	0.009412000	-0.373241000
6	0.956540000	-1.166423000	-0.193974000
6	-0.355774000	-0.789397000	-0.964715000

6	-0.362683000	0.788767000	-0.963213000
6	-1.593966000	1.127394000	-0.175706000
6	-1.582595000	-1.140005000	-0.175341000
6	-2.287247000	-0.009776000	0.261628000

MP2/cc-PVTZ solvent model ε_r=2:

$C_5Cl_5^+$trip MP2=-2488.3466052
Sum of electronic and thermal Free Energies= -2488.334168

17	0.882172000	-2.731963000	0.000000000
17	2.872876000	0.000000000	0.000000000
17	0.882172000	2.731964000	0.000000000
17	-2.318763000	1.694248000	0.000000000
17	-2.318763000	-1.694248000	0.000000000
6	0.375058000	-1.153740000	0.000000000
6	1.214979000	0.000000000	0.000000000
6	0.375058000	1.153739000	0.000000000
6	-0.982113000	0.713599000	0.000000000
6	-0.982113000	-0.713598000	0.000000000

$C_{10}Cl_{10}^{2+}$ MP2=-4976.7187775
Sum of electronic and thermal Free Energies= -4976.673239

17	-0.074440000	2.440957000	-2.681023000
17	-2.064628000	0.033339000	-1.597295000
17	-2.064617000	0.032857000	1.597078000
17	2.064628000	-0.033339000	-1.597295000
17	0.074440000	-2.440957000	-2.681023000
17	2.064617000	-0.032857000	1.597078000
17	0.599665000	4.271143000	0.000137000
17	-0.074793000	2.440789000	2.681109000
17	-0.599665000	-4.271143000	0.000137000
17	0.074793000	-2.440789000	2.681109000
6	0.074440000	2.685594000	0.000061000
6	-0.190005000	1.910208000	1.135570000
6	-0.189796000	1.910269000	-1.135530000
6	-0.605703000	0.515473000	0.782474000
6	-0.605644000	0.515541000	-0.782589000
6	0.605644000	-0.515541000	-0.782589000
6	0.605703000	-0.515473000	0.782474000
6	0.189796000	-1.910269000	-1.135530000
6	-0.074440000	-2.685594000	0.000061000
6	0.190005000	-1.910208000	1.135570000

$C_{10}Cl_{10}^{2+}$exo MP2=-4976.6979669
Sum of electronic and thermal Free Energies= -4976.654195

17	-2.825140000	-1.343139000	0.000000000
17	0.528115000	-3.345788000	1.693835000
17	0.528115000	-3.345788000	-1.693835000
17	-0.986055000	-0.735547000	2.752279000
17	-0.986055000	-0.735547000	-2.752279000
17	2.208977000	0.184622000	-1.538408000
17	2.208977000	0.184622000	1.538408000
17	0.000827000	2.376506000	2.667622000
17	0.000827000	2.376506000	-2.667622000
17	-0.705119000	4.159401000	0.000000000
6	0.271795000	-2.047819000	0.700623000
6	-0.315585000	-0.716405000	1.166813000
6	0.271795000	-2.047819000	-0.700623000
6	-0.315585000	-0.716405000	-1.166813000
6	-1.239141000	-0.931127000	0.000000000
6	0.647150000	0.441722000	0.789944000
6	0.647150000	0.441722000	-0.789944000
6	0.132594000	1.815296000	-1.134039000
6	0.132594000	1.815296000	1.134039000
6	-0.157597000	2.580636000	0.000000000

$C_{10}Cl_{10}^{2+}$endo MP2=-4976.6966016
Sum of electronic and thermal Free Energies= -4976.652572

17	1.549029000	2.766238000	-0.415668000
17	1.572459000	-2.751367000	-0.424270000
17	-0.419050000	1.525073000	-2.555681000
17	-0.414079000	-1.525135000	-2.556395000
17	-1.971988000	-2.690038000	0.171831000
17	-3.693835000	-0.014437000	1.143185000
17	-2.002453000	2.672061000	0.170345000
17	1.039125000	1.696463000	2.572443000
17	1.058225000	-1.695439000	2.566742000
17	3.501296000	0.017123000	-0.560688000
6	0.872458000	0.700004000	1.256006000
6	0.879590000	-0.695941000	1.253907000
6	0.942907000	1.173601000	-0.196336000
6	1.885535000	0.008949000	-0.356546000
6	0.953802000	-1.164612000	-0.200238000
6	-0.351900000	-0.786841000	-0.976253000
6	-0.358457000	0.786142000	-0.975604000
6	-1.584759000	1.125756000	-0.182903000
6	-1.573652000	-1.138736000	-0.181772000
6	-2.285252000	-0.009855000	0.242851000

MP2/cc-PVTZ solvent model ε_r=10:

$C_5Cl_5^+$trip MP2=-2488.3759556
Sum of electronic and thermal Free Energies= -2488.362671

17	0.884995000	-2.730536000	0.000000000
17	2.871241000	0.000000000	0.000000000
17	0.884995000	2.730536000	0.000000000
17	-2.320593000	1.690177000	0.000000000
17	-2.320593000	-1.690177000	0.000000000
6	0.374700000	-1.153176000	0.000000000
6	1.213287000	0.000000000	0.000000000
6	0.374700000	1.153176000	0.000000000
6	-0.981408000	0.712927000	0.000000000
6	-0.981408000	-0.712927000	0.000000000

$C_{10}Cl_{10}^{2+}$ MP2=-4976.810743
Sum of electronic and thermal Free Energies= -4976.766702

17	-0.006645000	2.464537000	-2.655515000
17	-2.049163000	0.059819000	-1.654013000
17	-2.071795000	-0.049659000	1.554649000
17	2.049163000	-0.059819000	-1.654013000
17	0.006645000	-2.464537000	-2.655515000
17	2.071795000	0.049659000	1.554649000
17	0.479603000	4.294004000	0.054895000
17	-0.166940000	2.401242000	2.697419000
17	-0.479603000	-4.294004000	0.054895000
17	0.166940000	-2.401242000	2.697419000
6	0.006645000	2.691349000	0.025201000
6	-0.254464000	1.894688000	1.143745000
6	-0.187495000	1.918065000	-1.123627000
6	-0.623699000	0.496436000	0.762991000
6	-0.603128000	0.515281000	-0.801040000
6	0.603128000	-0.515281000	-0.801040000
6	0.623699000	-0.496436000	0.762991000
6	0.187495000	-1.918065000	-1.123627000
6	-0.006645000	-2.691349000	0.025201000
6	0.254464000	-1.894688000	1.143745000

$C_{10}Cl_{10}^{2+}$exo MP2=-4976.791418
Sum of electronic and thermal Free Energies= -4976.748557

17	-2.829703000	-1.306050000	0.000000000
17	0.501607000	-3.354892000	1.678522000
17	0.501607000	-3.354892000	-1.678522000
17	-0.980756000	-0.723457000	2.754050000
17	-0.980756000	-0.723457000	-2.754050000
17	2.210411000	0.160324000	-1.554075000
17	2.210411000	0.160324000	1.554075000

17	0.040135000	2.386243000	2.663451000
17	0.040135000	2.386243000	-2.663451000
17	-0.745749000	4.136302000	0.000000000
6	0.257359000	-2.043974000	0.698962000
6	-0.316025000	-0.709453000	1.166467000
6	0.257359000	-2.043974000	-0.698962000
6	-0.316025000	-0.709453000	-1.166467000
6	-1.242802000	-0.913869000	0.000000000
6	0.659135000	0.440062000	0.790410000
6	0.659135000	0.440062000	-0.790410000
6	0.148858000	1.815835000	-1.133108000
6	0.148858000	1.815835000	1.133108000
6	-0.163319000	2.569982000	0.000000000

$C_{10}Cl_{10}^{2+}$endo MP2=-4976.7909901
Sum of electronic and thermal Free Energies= -4976.748572

17	2.272250000	2.159268000	-0.780331000
17	0.732461000	-3.077555000	-0.020779000
17	-0.190786000	1.434548000	-2.633450000
17	-0.661726000	-1.597922000	-2.441477000
17	-2.762894000	-2.074089000	0.073661000
17	-3.542592000	0.952280000	1.170471000
17	-1.175501000	3.045227000	0.152436000
17	1.637425000	1.642177000	2.341907000
17	0.560788000	-1.511218000	2.781797000
17	3.343647000	-1.021483000	-0.548388000
6	1.102835000	0.609645000	1.160433000
6	0.670238000	-0.704906000	1.339788000
6	1.241843000	0.857105000	-0.342671000
6	1.804678000	-0.537356000	-0.342333000
6	0.583318000	-1.363729000	-0.032031000
6	-0.558359000	-0.753037000	-0.919472000
6	-0.165268000	0.767910000	-1.019817000
6	-1.215296000	1.439574000	-0.181031000
6	-1.867019000	-0.730267000	-0.193246000
6	-2.200672000	0.553236000	0.258805000

MP2/cc-PVTZ solvent model ε_r=23:

$C_5Cl_5^+$trip MP2=-2488.3802615
Sum of electronic and thermal Free Energies= -2488.366842

17	0.000000000	2.730427000	0.885372000
17	0.000000000	0.000000000	2.871124000
17	0.000000000	-2.730427000	0.885372000
17	0.000000000	-1.689170000	-2.320973000
17	0.000000000	1.689170000	-2.320973000
6	0.000000000	1.153131000	0.374726000

6	0.000000000	0.000000000	1.213102000
6	0.000000000	-1.153131000	0.374726000
6	0.000000000	-0.712804000	-0.981165000
6	0.000000000	0.712804000	-0.981165000

$C_{10}Cl_{10}^{2+}$ MP2=-4976.824129
Sum of electronic and thermal Free Energies= -4976.780440

17	-0.019405000	2.455218000	-2.660658000
17	-2.052086000	0.047687000	-1.643158000
17	-2.068899000	-0.040453000	1.565687000
17	2.052086000	-0.047687000	-1.643158000
17	0.019405000	-2.455218000	-2.660658000
17	2.068899000	0.040453000	1.565687000
17	0.477962000	4.294219000	0.043710000
17	-0.146961000	2.405235000	2.693673000
17	-0.477962000	-4.294219000	0.043710000
17	0.146961000	-2.405235000	2.693673000
6	0.004984000	2.691184000	0.019825000
6	-0.247252000	1.896531000	1.141649000
6	-0.193983000	1.915109000	-1.125808000
6	-0.621776000	0.498112000	0.766825000
6	-0.605305000	0.513026000	-0.797039000
6	0.605305000	-0.513026000	-0.797039000
6	0.621776000	-0.498112000	0.766825000
6	0.193983000	-1.915109000	-1.125808000
6	-0.004984000	-2.691184000	0.019825000
6	0.247252000	-1.896531000	1.141649000

$C_{10}Cl_{10}^{2+}$ exo MP2=-4976.8052274
Sum of electronic and thermal Free Energies= -4976.762316

17	-2.832695000	-1.287951000	0.000000000
17	0.504414000	-3.356437000	1.676066000
17	0.504414000	-3.356437000	-1.676066000
17	-0.978589000	-0.726819000	2.754379000
17	-0.978589000	-0.726819000	-2.754379000
17	2.210918000	0.159981000	-1.555415000
17	2.210918000	0.159981000	1.555415000
17	0.040470000	2.385955000	2.662810000
17	0.040470000	2.385955000	-2.662810000
17	-0.752930000	4.132075000	0.000000000
6	0.257035000	-2.044535000	0.698321000
6	-0.315517000	-0.709958000	1.166096000
6	0.257035000	-2.044535000	-0.698321000
6	-0.315517000	-0.709958000	-1.166096000
6	-1.243685000	-0.909074000	0.000000000
6	0.660160000	0.439576000	0.790604000

6	0.660160000	0.439576000	-0.790604000
6	0.148606000	1.814830000	-1.132807000
6	0.148606000	1.814830000	1.132807000
6	-0.165812000	2.567507000	0.000000000

$C_{10}Cl_{10}^{2+}$endo MP2=-4976.8047703
Sum of electronic and thermal Free Energies= -4976.762677

17	2.275487000	2.154059000	-0.799243000
17	0.722566000	-3.073535000	-0.000123000
17	-0.210364000	1.443515000	-2.627633000
17	-0.638459000	-1.598406000	-2.446270000
17	-2.773824000	-2.077232000	0.038610000
17	-3.543527000	0.935222000	1.174186000
17	-1.160624000	3.032559000	0.189606000
17	1.657421000	1.650962000	2.329464000
17	0.546123000	-1.486190000	2.790326000
17	3.339732000	-1.031131000	-0.549206000
6	1.110508000	0.617176000	1.155111000
6	0.665654000	-0.692249000	1.342707000
6	1.244779000	0.856405000	-0.349586000
6	1.803709000	-0.539225000	-0.341264000
6	0.579358000	-1.359232000	-0.024758000
6	-0.557339000	-0.753353000	-0.922720000
6	-0.166455000	0.767623000	-1.017846000
6	-1.211751000	1.432096000	-0.167128000
6	-1.871850000	-0.734350000	-0.208590000
6	-2.201774000	0.544695000	0.258629000

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