# Design, Synthesis and Structural Characterization of a Bisantimony(III) Compound for Anion Binding and the Density Functional Theory Evaluation of Halide Binding through Antimony Secondary Bonding Interactions.

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**S1. IR and NMR Spectra of Compounds 1, 2, and 3**

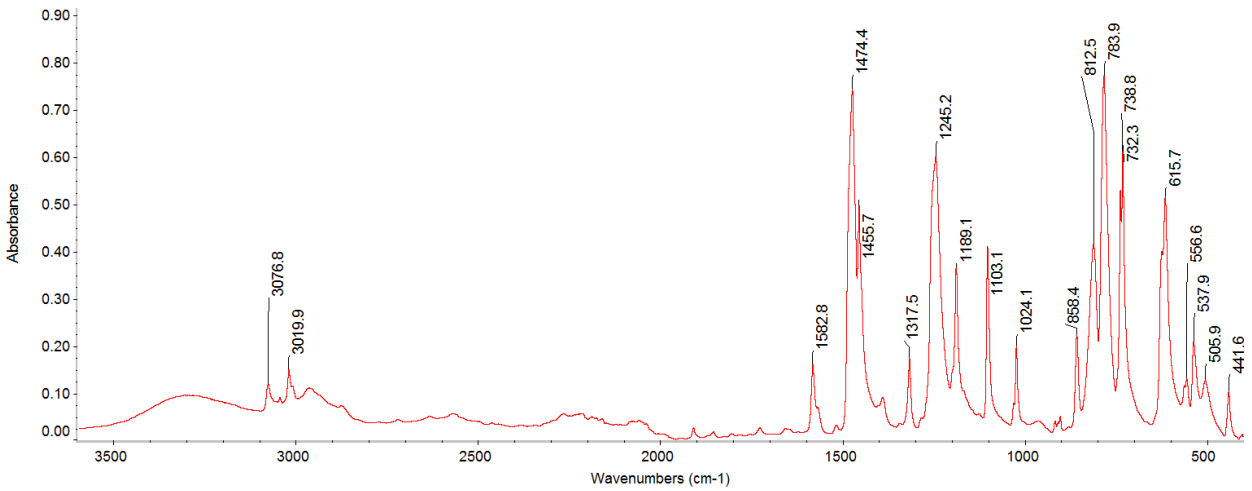


Figure S1. IR spectrum of **1**, $C_{12}H_8O_5Sb_2$.

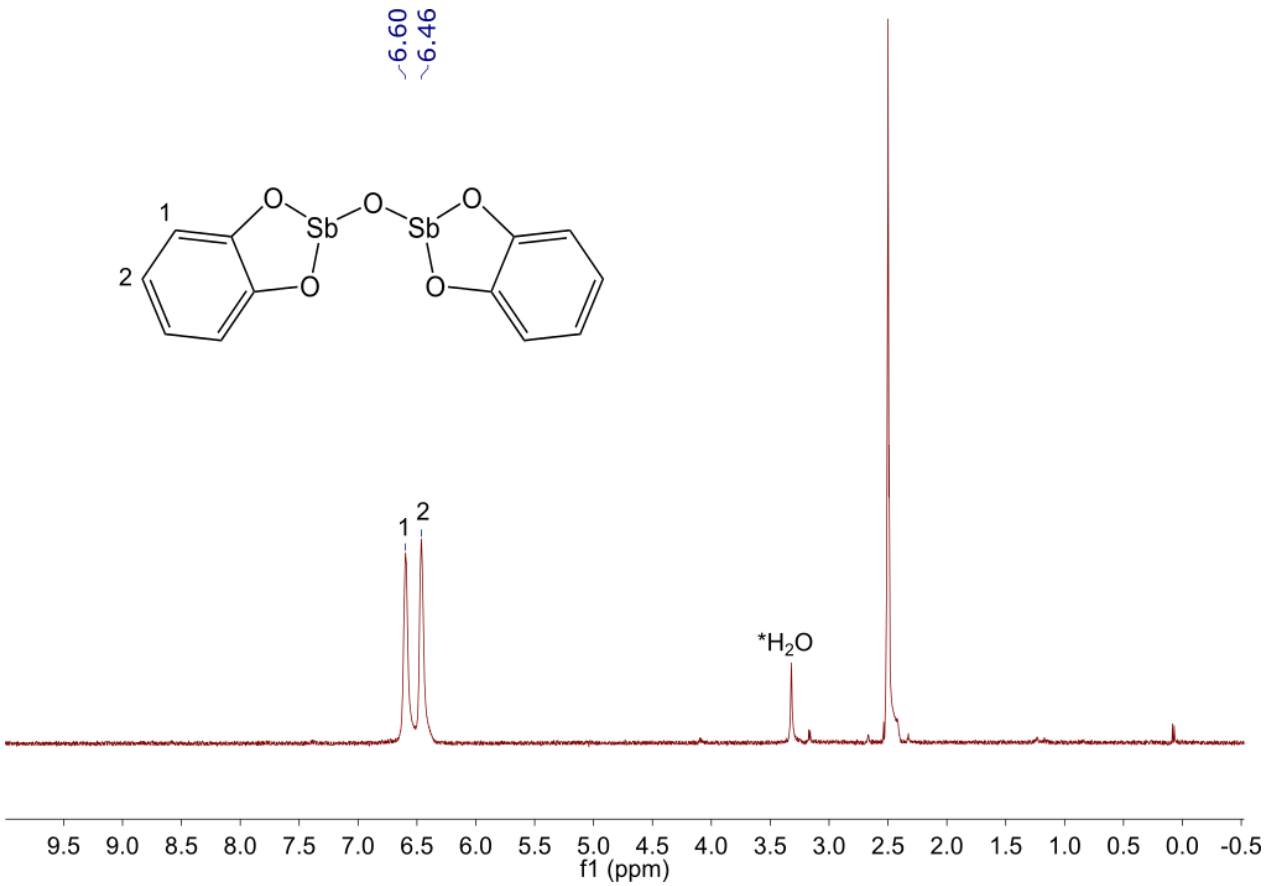


Figure S2. $^1$H NMR ($d_6$-DMSO) spectrum of **1**, $C_{12}H_8O_5Sb_2$.

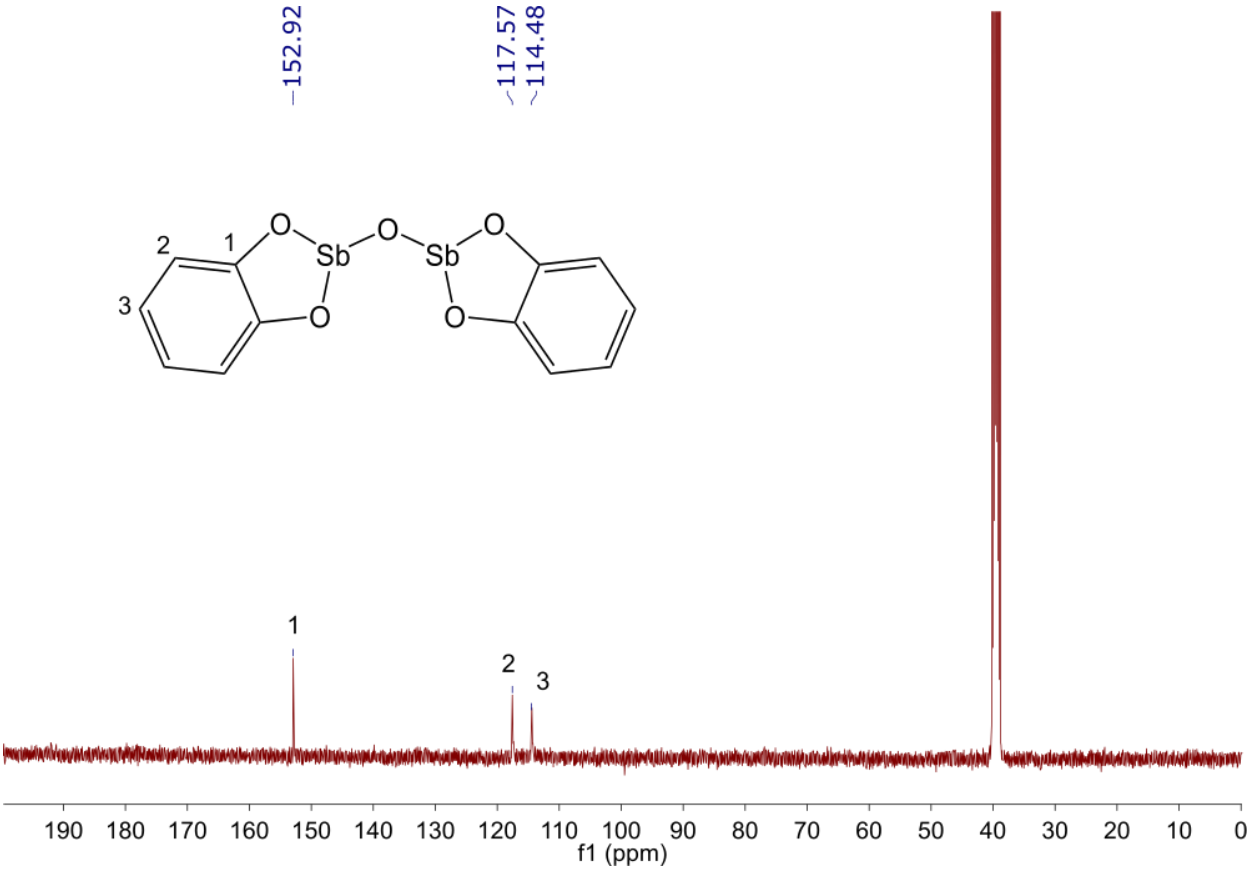


Figure S3. $^{13}C$ NMR ($d_6$-DMSO) spectrum of **1**, $C_{12}H_8O_5Sb_2$.

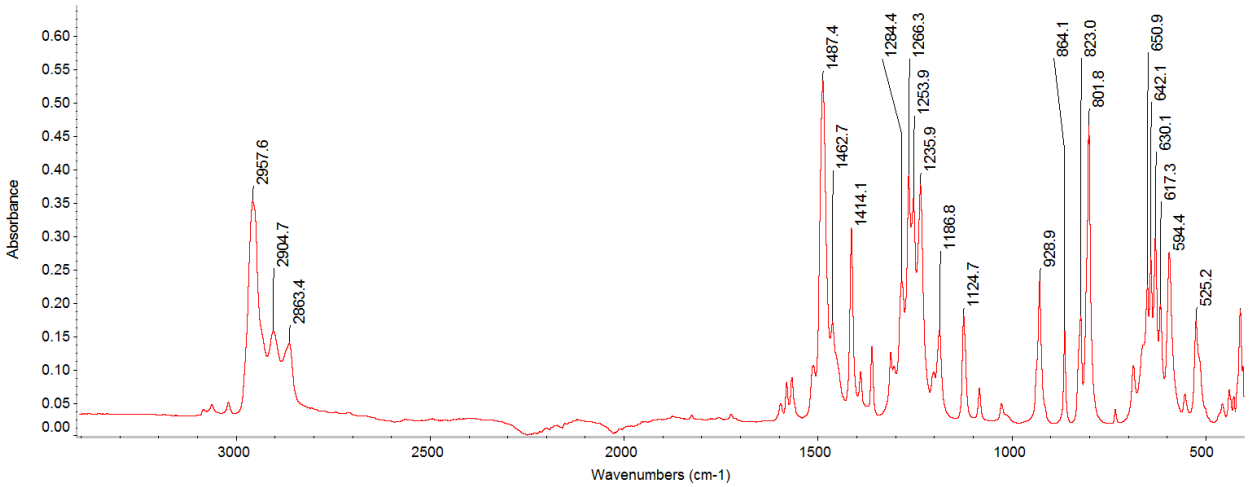


Figure S4. IR spectrum of **2**, $C_{20}H_{24}O_5Sb_2$.

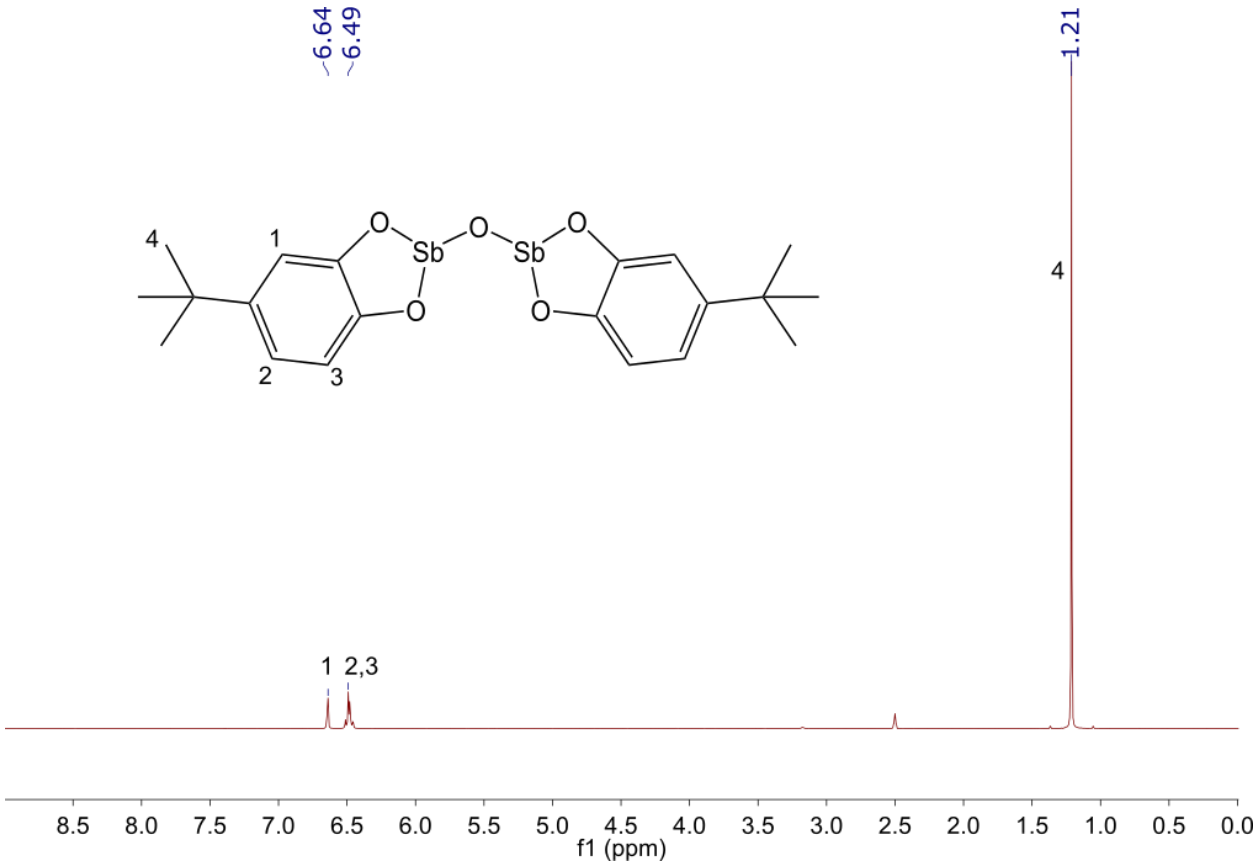


Figure S5. $^1$H NMR ($d_6$-DMSO) spectrum of **2**, $C_{20}H_{24}O_5Sb_2$.

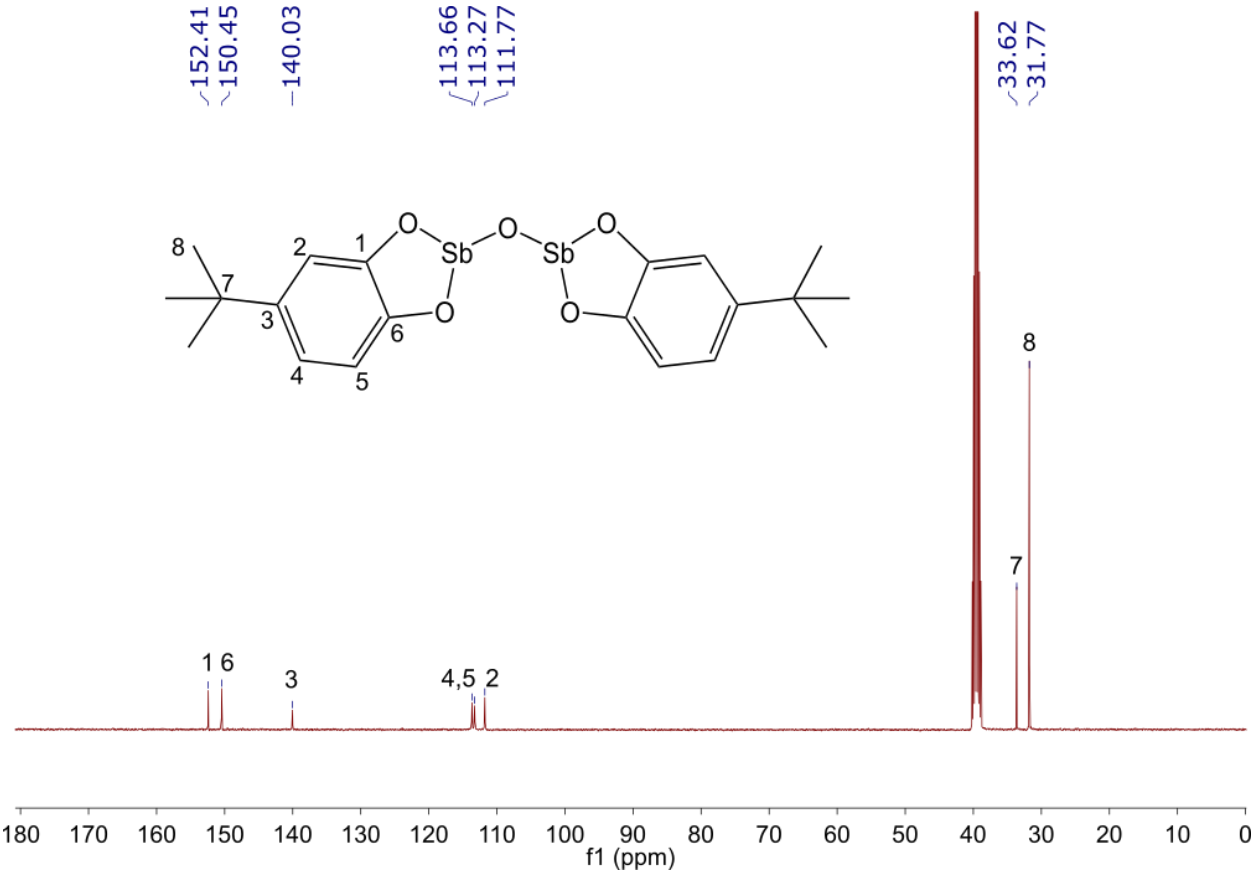


Figure S6. $^{13}C$ NMR ($d_6$-DMSO) spectrum of **2**, $C_{20}H_{24}O_5Sb_2$.

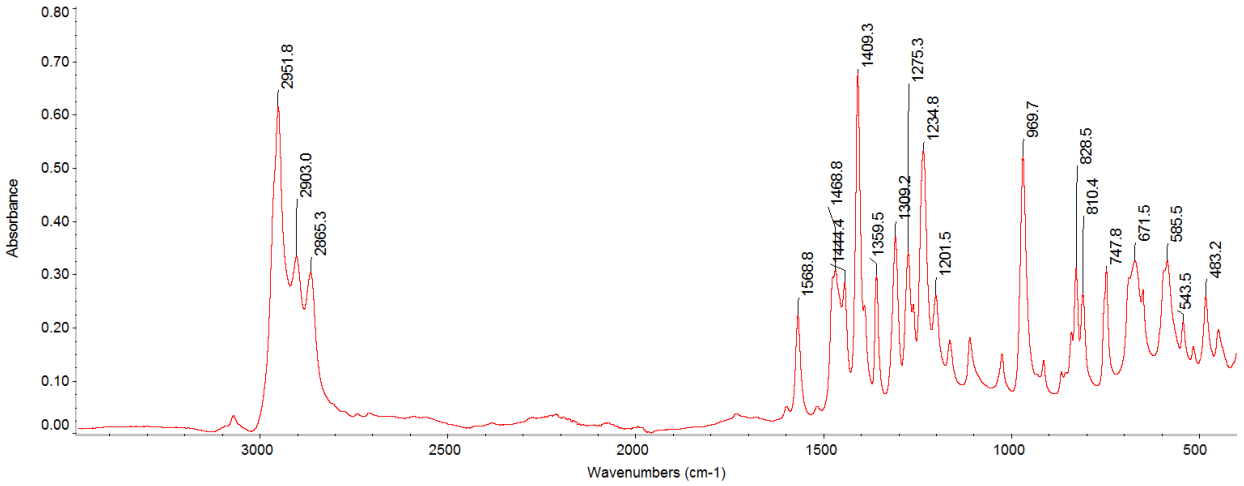


Figure S7. IR spectrum of **3**, $C_{28}H_{40}O_5Sb_2$.

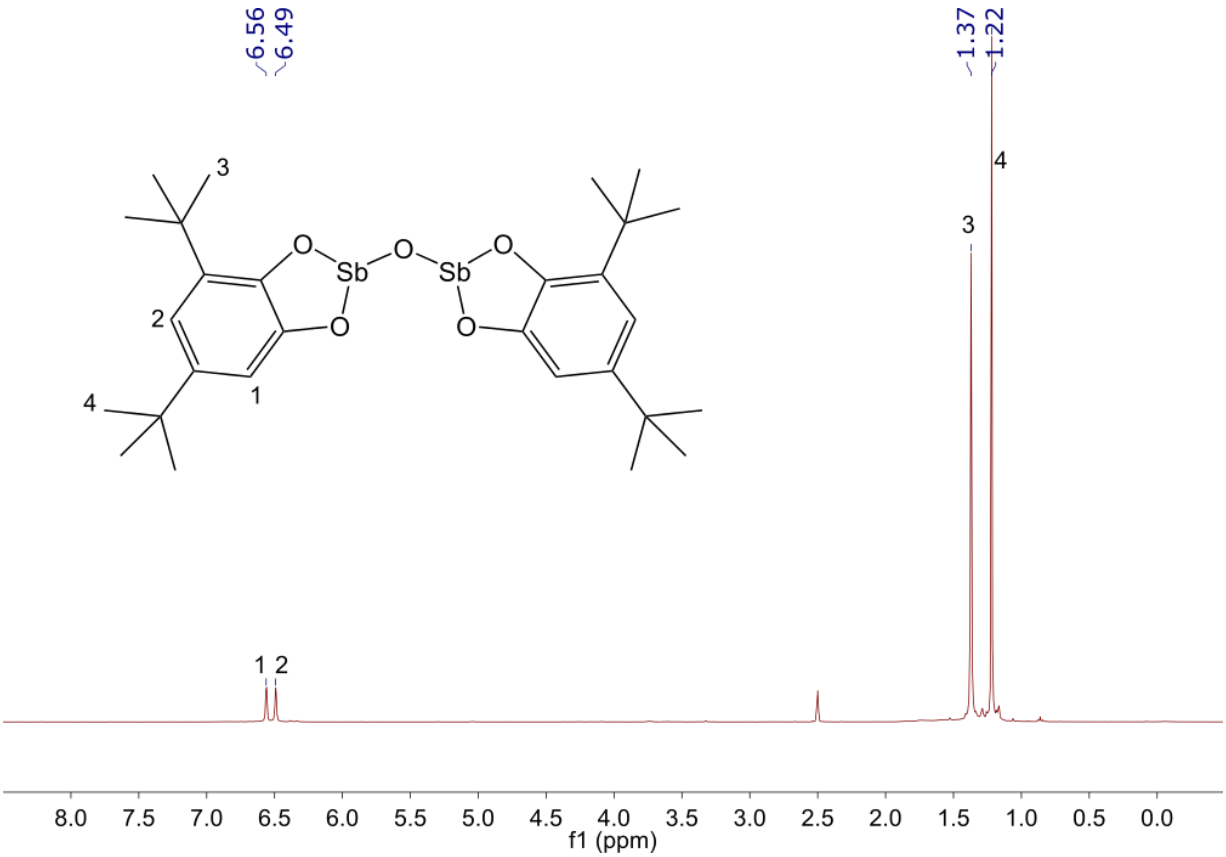


Figure S8. $^{1}$H NMR ($d_6$-DMSO) spectrum of **3**, $C_{28}H_{40}O_5Sb_2$.

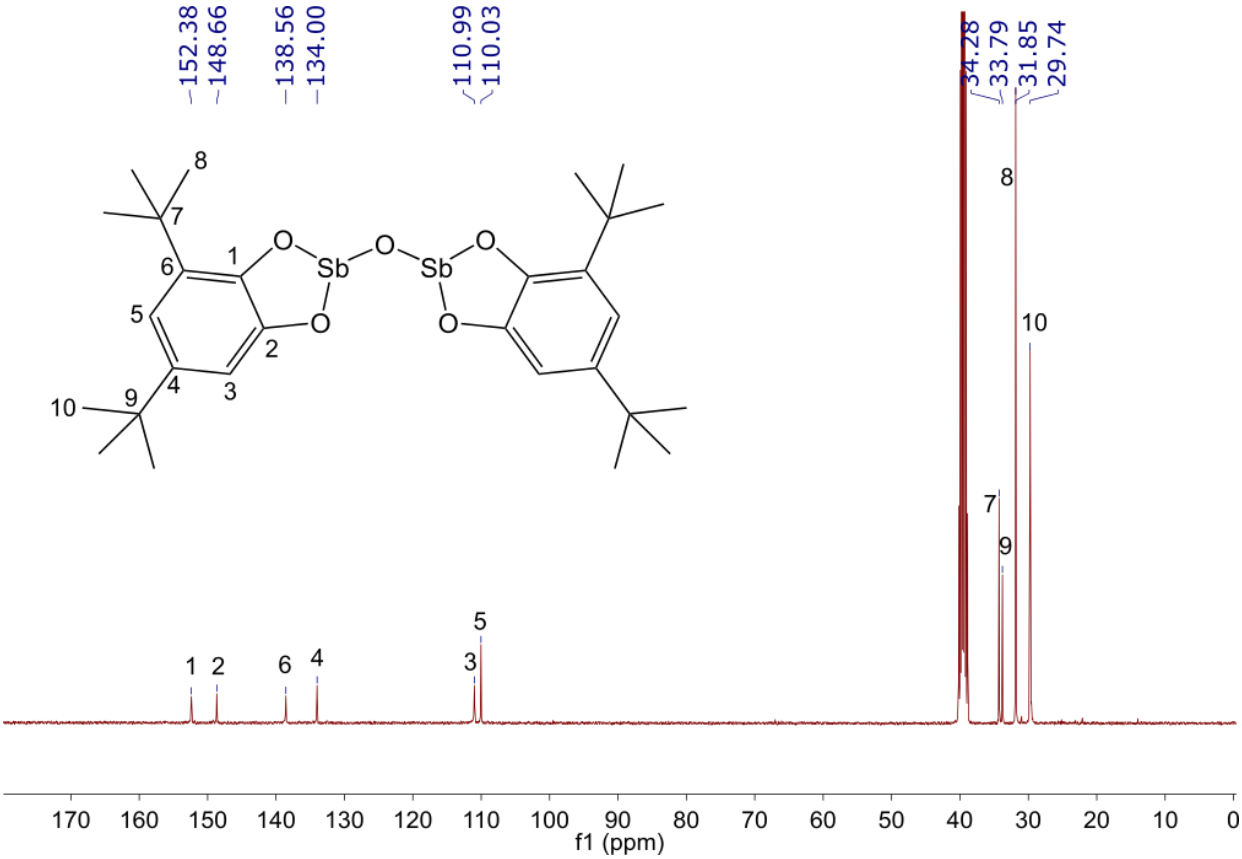


Figure S9. $^{13}$C NMR ($d_6$-DMSO) spectrum of **3**, $C_{28}H_{40}O_5Sb_2$.

**S2. Crystallographic Data**

Table S1. Crystal data and structure refinement for **3**·4Py.

| | |
|---|---|
| Empirical formula | $C_{48}H_{60}N_4O_5Sb_2$ |
| Formula weight | 1016.50 |
| Temperature | 100(2) K |
| Wavelength | 0.71073 Å |
| Crystal system, space group | Orthorhombic, *Pbca* |
| Unit cell dimensions | $a$ = 18.464(2) Å α = 90° |
| | $b$ = 17.963(2) Å β = 90° |
| | $c$ = 28.523(3) Å γ = 90° |
| Volume | 9460(2) Å$^3$ |
| Z, Calculated density | 8, 1.427 g/cm$^3$ |
| Absorption coefficient | 1.190 mm$^{-1}$ |
| F(000) | 4144 |
| Crystal size | 0.185 x 0.160 x 0.075 mm |
| Theta range for data collection | 1.428 to 27.160° |
| Limiting indices | $-23 \le h \le 23$, $-23 \le k \le 22$, $-36 \le l \le 36$ |
| Reflections collected / unique | 107391/10478 [$R$(int) = 0.0445] |
| Completeness to theta = 25.242° | 100.0 % |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 10478 / 522 / 545 |
| Goodness-of-fit on $F^2$ | 1.035 |
| Final R indices [I>2sigma(I)] | R1 = 0.0317, wR$^2$ = 0.0747 |
| R indices (all data) | R1 = 0.0500, wR$^2$ = 0.0867 |
| Extinction coefficient | n/a |
| Largest diff. peak and hole | 3.484 and -0.581 e·Å$^{-3}$ |

**S3. DFT Optimized Cartesian Coordinates**

Table S2. Cartesian coordinates (in Å) of $F_2SbOSbF_2$

| Atom | x | y | z |
|---|---|---|---|
| F | 1.36845155617254 | 1.81245621895065 | 0.04958086540346 |
| F | 2.06337912497476 | -0.33881056397363 | 1.68416413986885 |
| Sb | 0.60295274191364 | 0.92435514771972 | 1.62929913823362 |
| O | -0.52283340686162 | -0.12091704471187 | 0.47381283491747 |
| Sb | -0.25849421936662 | 0.06068507177420 | -1.48296644937059 |
| F | -1.29539852220752 | 1.68396035822803 | -1.58678381265747 |
| F | -1.78861927462518 | -1.07850918798708 | -1.76388571639533 |

Table S3. Cartesian coordinates (in Å) of $F_2SbOSbF_2 \cdot 1F^-$

| Atom | x | y | z |
|---|---|---|---|
| F | -0.02420378909523 | 1.41676217426989 | 2.03246720689115 |
| F | 2.55528048498388 | 0.92744986678011 | 1.11551650419566 |
| Sb | 0.89008636381386 | -0.15158336434415 | 1.32156044311621 |
| O | 0.56235303385702 | 0.12773072922643 | -0.59463303788440 |
| Sb | -1.13644831907973 | -0.61887320241796 | -1.23822483205387 |
| F | -0.71889940790130 | 0.17063987686361 | -3.02199262907632 |
| F | -2.31075404727494 | 0.88996493426408 | -0.85717009243987 |
| F | -1.19919231930355 | -1.04011101464199 | 1.01328043725144 |

Table S4. Cartesian coordinates (in Å) of $F_2SbOSbF_2 \cdot 2F^-$

| Atom | x | y | z |
|---|---|---|---|
| F | 0.52815056626315 | 1.76540030750232 | 2.36241775111575 |
| F | 2.72613273314857 | 0.62128615735697 | 0.92491689847911 |
| F | 1.24193816087683 | -1.72083299187596 | -0.04261029393469 |
| Sb | 0.87586831847942 | -0.03993198298410 | 1.39184040872660 |
| O | 0.05997289269558 | 0.73661261803520 | -0.23324417939923 |
| Sb | -0.93492505088811 | -0.69989856945576 | -1.15841573581198 |
| F | -0.37632277148701 | 0.15471814512844 | -2.96886081611645 |
| F | -2.64707277023577 | 0.36808767412073 | -1.23693008459668 |
| F | -1.47374607885265 | -1.18544135782783 | 0.96088305153758 |

Table S5. Cartesian coordinates (in Å) of $F_2SbOSbF_2 \cdot 1Cl^-$

| Atom | x | y | z |
|---|---|---|---|
| F | 0.03661201376482 | 1.48762163914797 | 2.00026158372732 |
| F | 2.61486328847555 | 0.98984717398740 | 1.03736893013220 |
| Sb | 0.96181474837168 | -0.08594038036033 | 1.32893804313121 |
| O | 0.53805096556216 | 0.15403969277669 | -0.56976867682265 |
| Sb | -1.11036615607903 | -0.57880595260610 | -1.33679557245868 |
| F | -0.58886238109919 | 0.22809894706713 | -3.08395243799574 |
| F | -2.26514326744481 | 0.94072295048616 | -0.96210648093837 |
| Cl | -1.56874721155117 | -1.41360407049892 | 1.35685861122472 |

Table S6. Cartesian coordinates (in Å) of $F_2SbOSbF_2 \cdot 2Cl^-$

| Atom | x | y | z |
|---|---|---|---|
| F | 0.32976713084696 | 1.68593329179124 | 2.44080886113339 |
| F | 2.63753884203376 | 1.00620509854847 | 0.94514290584512 |
| Cl | 1.49385559685915 | -2.18906331525652 | -0.48932434953571 |
| Sb | 0.91882304701472 | 0.05266552658965 | 1.40735634907223 |
| O | 0.05355720286600 | 0.73413768963470 | -0.23306634658416 |
| Sb | -0.96918272227006 | -0.64194161386586 | -1.21482432513287 |
| F | -0.18607760759967 | -0.03166631332096 | -2.97391055462749 |
| F | -2.50493640216500 | 0.64095433849141 | -1.48971150145021 |
| Cl | -1.77334908758584 | -1.25722470261214 | 1.60752596127969 |

Table S7. Cartesian coordinates (in Å) of $F_2SbOSbF_2 \cdot 1Br^-$

| Atom | x | y | z |
|---|---|---|---|
| F | 0.04664642448330 | 1.50695553537355 | 1.97790148016938 |
| F | 2.63140905105843 | 1.00781472820689 | 1.02076950380631 |
| Sb | 0.97954395521723 | -0.06698339095294 | 1.32142454020687 |
| O | 0.54361895710433 | 0.15801673221987 | -0.57490985140288 |
| Sb | -1.10215758473787 | -0.56174941541008 | -1.35607138912748 |
| F | -0.57200242439629 | 0.24559203271899 | -3.10023443663511 |
| F | -2.24422200290544 | 0.96362630809293 | -0.97183161925565 |
| Br | -1.66461437582371 | -1.53129253024923 | 1.45375577223854 |

Table S8. Cartesian coordinates (in Å) of $F_2SbOSbF_2 \cdot 2Br^-$

| Atom | x | y | z |
|---|---|---|---|
| F | 0.30273946780244 | 1.71634403170788 | 2.42793371481995 |
| F | 2.62369652196130 | 1.05200276203167 | 0.96646277732017 |
| Br | 1.60308747847812 | -2.32015347821945 | -0.51264885708966 |
| Sb | 0.91584640780213 | 0.08730824030995 | 1.41712012900127 |
| O | 0.05917766885783 | 0.73863720778865 | -0.23861487303366 |
| Sb | -0.96070176058186 | -0.62129693339242 | -1.24343293643317 |
| F | -0.15804248167007 | -0.00358486733257 | -2.98278081136667 |
| F | -2.48152894154140 | 0.66639032225180 | -1.52798483663371 |
| Br | -1.90427836110849 | -1.31564728514554 | 1.69394269341547 |

Table S9. Cartesian coordinates (in Å) of $F_2SbOSbF_2 \cdot 1I^-$

| Atom | x | y | z |
|---|---|---|---|
| F | 0.07571274332529 | 1.51027931448899 | 1.98956599640405 |
| F | 2.65404298062907 | 1.01556475900274 | 1.01736976575301 |
| Sb | 0.99858620365704 | -0.06278197068416 | 1.31377017823072 |
| O | 0.52801278357399 | 0.20014977267951 | -0.57112007505839 |
| Sb | -1.09220524394476 | -0.55834956903520 | -1.37297731093460 |
| F | -0.56317241100317 | 0.24712015028050 | -3.12319349773462 |
| F | -2.24747872596114 | 0.96221287905091 | -1.00432580258581 |
| I | -1.73527633027631 | -1.59221533578330 | 1.52171474592563 |

Table S10. Cartesian coordinates (in Å) of $F_2SbOSbF_2 \cdot 2I^-$

| Atom | x | y | z |
|---|---|---|---|
| F | 0.28430449351181 | 1.75341739168192 | 2.41715391027427 |
| F | 2.63694081097866 | 1.07796572480843 | 0.93995541789085 |
| I | 1.54161893706636 | -2.41009663642596 | -0.44467103827465 |
| Sb | 0.92367739052643 | 0.11555952279508 | 1.41794163936113 |
| O | 0.06217030151337 | 0.76023917631920 | -0.24659681126479 |
| Sb | -0.96384250561404 | -0.59797259967196 | -1.26158949009791 |
| F | -0.13608724188249 | 0.03057991271852 | -2.99626448081470 |
| F | -2.48930371895048 | 0.70452800315692 | -1.52010067993626 |
| I | -1.85948246714961 | -1.43422049538218 | 1.69416853286208 |

Table S11. Cartesian coordinates (in Å) of $Cl_2SbOSbCl_2$

| Atom | x | y | z |
|---|---|---|---|
| Cl | 1.75050630925020 | 2.48383717777743 | 1.66715801722607 |
| Cl | 1.36876975343297 | -1.04497551204193 | 1.82845017011535 |
| Sb | 0.11240542355183 | 0.84714084237489 | 1.10538240702540 |
| O | 0.79607766588392 | 0.72057231135751 | -0.76245676865689 |
| Sb | -0.29692041909333 | -0.15663113606189 | -2.09161621659468 |
| Cl | -1.96774772983435 | 1.55566609999079 | -2.23446445142196 |
| Cl | -1.59365300319126 | -1.46238978339679 | -0.50923215769329 |

Table S12. Cartesian coordinates (in Å) of $Cl_2SbOSbCl_2 \cdot 1F^-$

| Atom | x | y | z |
|---|---|---|---|
| Cl | -0.23833297570987 | 1.66881127056682 | 2.28374827318595 |
| Cl | 3.06568847492284 | 0.96267770164132 | 1.14062521655150 |
| Sb | 0.87880330695661 | -0.26406074378266 | 1.35186799743703 |
| O | 0.52673805082384 | 0.06610121976710 | -0.55454575441385 |
| Sb | -1.14680945293521 | -0.73319837678145 | -1.20864494227276 |
| Cl | -0.62320338795471 | 0.10700188407504 | -3.52201418980961 |
| Cl | -2.64706453534099 | 1.11095016830185 | -0.76148727639976 |
| F | -1.19759748076251 | -1.19630312378802 | 1.04125467572152 |

Table S13. Cartesian coordinates (in Å) of $Cl_2SbOSbCl_2 \cdot 2F^-$

| Atom | x | y | z |
|---|---|---|---|
| Cl | 0.17296281457606 | 1.78155481254202 | 2.91696301493168 |
| Cl | 3.20888565736259 | 0.90204008685142 | 0.79692447143774 |
| F | 1.00482852692833 | -1.81143881404204 | -0.33089908851211 |
| Sb | 0.90201997381840 | -0.16942965708552 | 1.35903534824309 |
| O | 0.05383011183923 | 0.68621725638129 | -0.21614179270400 |
| Sb | -0.97625124547714 | -0.78498335461479 | -1.05756826512709 |
| Cl | -0.04871323429850 | -0.19793226926175 | -3.41532751075742 |
| Cl | -3.08190925251839 | 0.72874466736090 | -1.31310630067847 |
| F | -1.23565735223057 | -1.13477272813154 | 1.26011712316659 |

Table S14. Cartesian coordinates (in Å) of $Cl_2SbOSbCl_2 \cdot 1Cl^-$

| Atom | x | y | z |
|---|---|---|---|
| Cl | -0.18712915426042 | 1.73716651342571 | 2.22940027134221 |
| Cl | 3.11191516547809 | 1.02048407985017 | 1.06590794344099 |
| Sb | 0.94256733636333 | -0.20911803117278 | 1.35523125207863 |
| O | 0.51876296292929 | 0.07938234034278 | -0.54286880241405 |
| Sb | -1.12349300335566 | -0.69989481520065 | -1.29236793717630 |
| Cl | -0.50601798451473 | 0.16294106363860 | -3.56739924267784 |
| Cl | -2.58941797159106 | 1.16569073519250 | -0.84668632951922 |
| Cl | -1.54896535104885 | -1.53467188607633 | 1.36958684492556 |

Table S15. Cartesian coordinates (in Å) of $Cl_2SbOSbCl_2 \cdot 2Cl^-$

| Atom | x | y | z |
|---|---|---|---|
| Cl | 0.15586257958374 | 1.93660394584038 | 2.81906858311606 |
| Cl | 3.14609695653775 | 1.05225974715885 | 0.82404956438379 |
| Cl | 1.38125426543369 | -2.22291533622220 | -0.43248149296536 |
| Sb | 0.91786019643179 | -0.07557065769843 | 1.41693833027122 |
| O | 0.04947698156359 | 0.65437502641939 | -0.20889320146378 |
| Sb | -0.98283338615056 | -0.75227728345133 | -1.14997734499248 |
| Cl | -0.00710474856800 | -0.05774780584526 | -3.42088280836875 |
| Cl | -3.00244922590897 | 0.80827723734827 | -1.42674579254353 |
| Cl | -1.65816761892303 | -1.34300487354968 | 1.57892116256281 |

Table S16. Cartesian coordinates (in Å) of $Cl_2SbOSbCl_2 \cdot 1Br^-$

| Atom | x | y | z |
|---|---|---|---|
| Cl | -0.19073846073121 | 1.73576214278243 | 2.21909495826855 |
| Cl | 3.11928903407324 | 1.05648619888651 | 1.05564782947006 |
| Sb | 0.96252025166151 | -0.19525874308693 | 1.34472659215277 |
| O | 0.52967671361563 | 0.09162168423957 | -0.55147957066657 |
| Sb | -1.10533223393538 | -0.68696501308530 | -1.31676018981824 |
| Cl | -0.48573641185246 | 0.19903506837246 | -3.58216752580491 |
| Cl | -2.57615712583157 | 1.16847921737254 | -0.85126414688918 |
| Br | -1.63529976699975 | -1.64718055548127 | 1.45300605328752 |

Table S17. Cartesian coordinates (in Å) of $Cl_2SbOSbCl_2 \cdot 2Br^-$

| Atom | x | y | z |
|---|---|---|---|
| Cl | 0.12013705352694 | 1.97415989633352 | 2.79185491275953 |
| Cl | 3.12540485487975 | 1.09579447928599 | 0.85221397662293 |
| Br | 1.48212928860980 | -2.35408909287310 | -0.44600796853126 |
| Sb | 0.91019361071553 | -0.04329327338488 | 1.43299004918363 |
| O | 0.05280773138521 | 0.65675986846142 | -0.21184420515700 |
| Sb | -0.97469151482050 | -0.73494077374294 | -1.18000940822505 |
| Cl | 0.04229402320556 | -0.03535080074998 | -3.41925141453856 |
| Cl | -2.96628370441422 | 0.84080077035431 | -1.48522244476042 |
| Br | -1.79199534308807 | -1.39984107368432 | 1.66527350264620 |

Table S18. Cartesian coordinates (in Å) of $Cl_2SbOSbCl_2 \cdot 1I^-$

| Atom | x | y | z |
|---|---|---|---|
| Cl | -0.17349989117611 | 1.73350633350585 | 2.21894659226534 |
| Cl | 3.13610655565801 | 1.06748458115789 | 1.03463564267101 |
| Sb | 0.98296992642178 | -0.19642176441671 | 1.33809023039154 |
| O | 0.51887705303353 | 0.11429753405439 | -0.54786094829655 |
| Sb | -1.09483654227923 | -0.68983110021808 | -1.33431495802210 |
| Cl | -0.46239031896832 | 0.21198443610007 | -3.59508237518342 |
| Cl | -2.57161426022923 | 1.16427793423112 | -0.86743951120719 |
| I | -1.71739052246044 | -1.68331795441454 | 1.52382932738137 |

Table S19. Cartesian coordinates (in Å) of $Cl_2SbOSbCl_2 \cdot 2I^-$

| Atom | x | y | z |
|---|---|---|---|
| Cl | 0.03634664419681 | 2.00864362105860 | 2.76596703177460 |
| Cl | 3.11973391542170 | 1.12314894616561 | 0.82786388422769 |
| I | 1.47119423107735 | -2.45770334106170 | -0.38219488769143 |
| Sb | 0.90134533419868 | -0.00474740313164 | 1.43828442545561 |
| O | 0.05593279612606 | 0.68829685745966 | -0.22264273878660 |
| Sb | -0.96105879188812 | -0.70898023749498 | -1.20592746377599 |
| Cl | 0.13135485073418 | -0.00691710777655 | -3.41435866338232 |
| Cl | -2.95441904197983 | 0.87778200427220 | -1.48085576077833 |
| I | -1.80043393788683 | -1.51952333949123 | 1.67386117295676 |

Table S20. Cartesian coordinates (in Å) of $Br_2SbOSbBr_2$

| Atom | x | y | z |
|---|---|---|---|
| Br | 1.72075058154950 | 2.65203573902805 | 1.62697657753887 |
| Br | 1.41017056789958 | -1.11159752664198 | 1.98467205353277 |
| Sb | 0.08583250624484 | 0.81878394141735 | 1.05597313306382 |
| O | 0.86502606965657 | 0.60823765826683 | -0.78116464314488 |
| Sb | -0.27861012687661 | -0.15301089883814 | -2.14996331354407 |
| Br | -1.97306494140012 | 1.73446895761306 | -2.18255699888230 |
| Br | -1.66066665707377 | -1.60569787084517 | -0.55071580856420 |

Table S21. Cartesian coordinates (in Å) of $Br_2SbOSbBr_2 \cdot 1F^-$

| Atom | x | y | z |
|---|---|---|---|
| Br | -0.28851963418943 | 1.73608888837297 | 2.39558548225004 |
| Br | 3.22005067555311 | 0.96525645929970 | 1.12852544888380 |
| Sb | 0.87788835257870 | -0.29124592543472 | 1.36351887857050 |
| O | 0.50365695885540 | 0.07711573447506 | -0.53873750179060 |
| Sb | -1.15506103406955 | -0.76089011380341 | -1.20270351592963 |
| Br | -0.57484797005901 | 0.07890353181237 | -3.66821337237889 |
| Br | -2.77386595585139 | 1.16637599639870 | -0.75407379111019 |
| F | -1.19107939281783 | -1.24962457112066 | 1.04690237150500 |

Table S22. Cartesian coordinates (in Å) of $Br_2SbOSbBr_2 \cdot 2F^-$

| Atom | x | y | z |
|---|---|---|---|
| Br | 0.15208270150343 | 1.88184072255792 | 3.02755012455948 |
| Br | 3.35967136952567 | 0.87857257445284 | 0.75408807532583 |
| F | 1.00062748146890 | -1.82762998857785 | -0.29945370103922 |
| Sb | 0.89761995661507 | -0.19472907908164 | 1.36533212480326 |
| O | 0.05038718095999 | 0.66774596417895 | -0.20959148790178 |
| Sb | -0.97745295151596 | -0.80994143684655 | -1.04872514822833 |
| Br | -0.01197077048702 | -0.18151415359677 | -3.55975565658339 |
| Br | -3.23368917915271 | 0.75326676665410 | -1.27250978387521 |
| F | -1.23727978891735 | -1.16761136974101 | 1.24306245293937 |

Table S23. Cartesian coordinates (in Å) of $Br_2SbOSbBr_2 \cdot 1Cl^-$

| Atom | x | y | z |
|---|---|---|---|
| Br | -0.23843586623366 | 1.81452013073064 | 2.33744530133825 |
| Br | 3.26713259937353 | 1.01598461162692 | 1.05145035362894 |
| Sb | 0.93700842247518 | -0.23336249563324 | 1.37045567363929 |
| O | 0.49427225135971 | 0.08581085723513 | -0.52515672310608 |
| Sb | -1.13601871898582 | -0.72542400666147 | -1.28385463289582 |
| Br | -0.45119061094480 | 0.13126344336876 | -3.71133159064793 |
| Br | -2.71848003058421 | 1.22627088666161 | -0.83965388986295 |
| Cl | -1.53606604645995 | -1.59308342732837 | 1.37144950790629 |

Table S24. Cartesian coordinates (in Å) of $Br_2SbOSbBr_2 \cdot 2Cl^-$

| Atom | x | y | z |
|---|---|---|---|
| Br | 0.09491154359917 | 2.01270930955189 | 2.92516541977443 |
| Br | 3.28885682182797 | 1.07486790095061 | 0.80145752955724 |
| Cl | 1.35997298530852 | -2.24828985487294 | -0.41325637711803 |
| Sb | 0.91625642391834 | -0.10614935627911 | 1.42547239246941 |
| O | 0.04965466780837 | 0.62870791503720 | -0.20223293429589 |
| Sb | -0.98514933892214 | -0.78252068657809 | -1.13915508100090 |
| Br | 0.05541325511961 | -0.06634955621543 | -3.55387983548608 |
| Br | -3.13769754597614 | 0.85991265386779 | -1.42151540767765 |
| Cl | -1.64222281268369 | -1.37288832546195 | 1.57794129377748 |

Table S25. Cartesian coordinates (in Å) of $Br_2SbOSbBr_2 \cdot 1Br^-$

| Atom | x | y | z |
|---|---|---|---|
| Br | -0.24055801742700 | 1.81378329736336 | 2.32942597053038 |
| Br | 3.27855826800781 | 1.04958225699563 | 1.04415199284340 |
| Sb | 0.95586910734885 | -0.21868090971003 | 1.35964255376001 |
| O | 0.50332602380828 | 0.10155467765658 | -0.53339666687894 |
| Sb | -1.11857603618213 | -0.71125575973858 | -1.30791921289669 |
| Br | -0.43171368372220 | 0.16508112158958 | -3.72950756726931 |
| Br | -2.70699704715876 | 1.22931472649893 | -0.84553579734592 |
| Br | -1.62168661467486 | -1.70739941065549 | 1.45394272725708 |

Table S26. Cartesian coordinates (in Å) of $Br_2SbOSbBr_2 \cdot 2Br^-$

| Atom | x | y | z |
|---|---|---|---|
| Br | 0.05753046112766 | 2.05257188948821 | 2.89966859972482 |
| Br | 3.26984528576777 | 1.11466433200686 | 0.82919753416460 |
| Br | 1.46360565845104 | -2.37576423224701 | -0.42641909634901 |
| Sb | 0.90720790854765 | -0.07439531423501 | 1.44196200042419 |
| O | 0.05200446531832 | 0.63186522676575 | -0.20498398694787 |
| Sb | -0.97640959784032 | -0.76625500190497 | -1.16933884294751 |
| Br | 0.10952834353066 | -0.04467730124118 | -3.55217411690173 |
| Br | -3.10473391202969 | 0.89052454379260 | -1.47974338341571 |
| Br | -1.77858261287309 | -1.42853414242525 | 1.66182829224822 |

Table S27. Cartesian coordinates (in Å) of $Br_2SbOSbBr_2 \cdot 1I^-$

| Atom | x | y | z |
|---|---|---|---|
| Br | -0.22520020850514 | 1.81232842131407 | 2.32154210179431 |
| Br | 3.29283144951320 | 1.06291576982366 | 1.02074140530094 |
| Sb | 0.97586863572107 | -0.22189876973695 | 1.35544915782551 |
| O | 0.49245222328773 | 0.11473302710928 | -0.52772225561787 |
| Sb | -1.10977347689285 | -0.71650964306525 | -1.32510136743071 |
| Br | -0.40677160356567 | 0.17951296725506 | -3.74068654215470 |
| Br | -2.69509343548072 | 1.22824902417878 | -0.85875544429945 |
| I | -1.70609158407764 | -1.73735079687867 | 1.52533694458194 |

Table S28. Cartesian coordinates (in Å) of $Br_2SbOSbBr_2 \cdot 2I^-$

| Atom | x | y | z |
|---|---|---|---|
| Br | -0.02933950708939 | 2.07677578218295 | 2.87771321148715 |
| Br | 3.26466510600895 | 1.13133435406383 | 0.80836227563583 |
| I | 1.48269549160248 | -2.46217974478477 | -0.38941336127797 |
| Sb | 0.89629144651173 | -0.04073258362076 | 1.44595394339481 |
| O | 0.05451531096533 | 0.66495179425343 | -0.21569488601704 |
| Sb | -0.96170295329560 | -0.74335599643164 | -1.19134318931206 |
| Br | 0.20115854674770 | -0.02742049268380 | -3.54273116720007 |
| Br | -3.09556915040037 | 0.91666169420364 | -1.47384713090832 |
| I | -1.81271829105082 | -1.51603480718289 | 1.68099730419766 |

Table S29. Cartesian coordinates (in Å) of **1**

| Atom | x | y | z |
|---|---|---|---|
| Sb | -2.13513687722788 | 6.40111800363352 | 5.04756033327604 |
| Sb | -1.23829225248904 | 5.50154404655171 | 2.24409114445120 |
| O | -2.04309218383268 | 7.06694555302052 | 3.17439866976179 |
| O | -0.32854502117955 | 5.44693471218102 | 4.67736592301690 |
| O | -0.90685794296031 | 7.84967623437028 | 5.72689456449935 |
| O | -2.37027957908905 | 4.30890158659521 | 3.51319804753169 |
| O | -2.84337425850309 | 5.25876453383990 | 1.04766944052988 |
| C | 0.70112256861984 | 6.35821110344892 | 4.81179321572426 |
| C | 2.02416630771970 | 6.01746227379314 | 4.55002842856098 |
| C | 3.02529686685396 | 6.97934329476363 | 4.71298564943580 |
| C | 2.70556500678381 | 8.24803114989783 | 5.20057909398544 |
| C | 1.38338136849443 | 8.58215995433113 | 5.50068870111889 |
| C | 0.38036089734152 | 7.62994058145021 | 5.33228109539424 |
| C | -3.90333465882045 | 4.74642073524494 | 1.73709823154302 |
| C | -5.17072685421288 | 4.62835588699995 | 1.17026192922003 |
| C | -6.18792260506262 | 3.99089696058161 | 1.88366056186331 |
| C | -5.93507524896846 | 3.44371251843090 | 3.14312353056571 |
| C | -4.66544677856243 | 3.55603748176626 | 3.71696937433603 |
| C | -3.65731617893828 | 4.21506109756187 | 3.02090936038014 |
| H | 2.25521131009480 | 5.02113460241463 | 4.17335703994391 |
| H | 4.05997455119716 | 6.72084776380055 | 4.48966869848849 |
| H | 3.48759633699771 | 8.99488751819723 | 5.33539153866886 |
| H | 1.11778842895372 | 9.56040983095012 | 5.89950015983314 |
| H | -5.34294767580480 | 5.04140051789238 | 0.17720467576671 |
| H | -7.17812643890189 | 3.90055461794107 | 1.43747796111626 |
| H | -6.72974998973097 | 2.94278342122836 | 3.69495908826443 |
| H | -4.44737809877229 | 3.12801201911311 | 4.69546854272348 |

Table S30. Cartesian coordinates (in Å) of $\mathbf{1}_2 \cdot F^-$

| Atom | x | y | z |
|---|---|---|---|
| Sb | -2.22993579588350 | 9.59239634692038 | 2.51065548917081 |
| Sb | 0.15398631829772 | 7.25104427979041 | 2.61498090641016 |
| O | -0.34624400228472 | 9.10869460871164 | 2.13092831381545 |
| O | -2.03017477506362 | 9.11309104905056 | 4.52800527154582 |
| O | -1.77166882032796 | 11.44672385889030 | 3.26530228805720 |
| O | -0.78336523508523 | 6.41191241302241 | 0.96746550467487 |
| O | 1.73965322809816 | 7.22346118293978 | 1.30964903320921 |
| C | -1.62896463981409 | 10.18096962509900 | 5.26336356281540 |
| C | -1.31972980273054 | 10.08306971448150 | 6.61787891389468 |
| C | -0.92390374199617 | 11.22379282004600 | 7.32525249246011 |
| C | -0.79207919430210 | 12.44668625020230 | 6.66609184401107 |
| C | -1.07594297410982 | 12.54575862611970 | 5.29955533694106 |
| C | -1.47778416137724 | 11.41667774396890 | 4.58635529199903 |
| C | 1.39333696997255 | 6.75393394869957 | 0.08609787191904 |
| C | 2.29806966748435 | 6.66477552564580 | -0.97165770848262 |
| C | 1.87846650583716 | 6.16495253824596 | -2.20929654998410 |
| C | 0.56052570175323 | 5.74251438379421 | -2.38799412660455 |
| C | -0.35471546840427 | 5.83432623554853 | -1.33349595793240 |
| C | 0.05926512356990 | 6.31019442349796 | -0.09153002671349 |
| H | -1.42008152387697 | 9.11679301349399 | 7.11313961286251 |
| H | -0.69064977572695 | 11.14105015295890 | 8.38742158193450 |
| H | -0.48077440407678 | 13.33599577666010 | 7.21610379234702 |
| H | -0.97134526181398 | 13.49135498628240 | 4.76713229970218 |
| H | 3.32157141420051 | 7.00602217110305 | -0.81451150173881 |
| H | 2.59346043926036 | 6.09783055310674 | -3.03066449860597 |
| H | 0.22920596191253 | 5.36212475290007 | -3.35507856793853 |
| H | -1.39068182268162 | 5.51764803220027 | -1.45697078719816 |
| F | -2.30775928204433 | 7.21845137137433 | 2.89352079280773 |
| Sb | -3.82051514364964 | 6.90881025579322 | 4.83194751576667 |
| Sb | -3.03023025173913 | 5.04028602764331 | 2.17969036978949 |
| O | -4.25587304338010 | 5.33219895527470 | 3.70868308300833 |
| O | -4.59638066740619 | 8.26094957308597 | 3.46163006764423 |
| O | -5.73260789401986 | 7.06796119363725 | 5.56566323545461 |
| O | -1.36259746521118 | 4.94328825942810 | 3.42314047403533 |
| O | -2.92135098818133 | 3.00828357919474 | 2.45439936598596 |
| C | -5.90257260275982 | 8.53359329713689 | 3.70979925296411 |
| C | -6.66012868141073 | 9.36881188822580 | 2.89189500372564 |
| C | -8.00261785287767 | 9.61745620697962 | 3.19847784054360 |
| C | -8.59623232693687 | 8.99539094113805 | 4.29758935954818 |
| C | -7.84928465847685 | 8.13631111203589 | 5.11108375107926 |

| | | | |
|---|---|---|---|
| C | -6.50892036344241 | 7.88798725829152 | 4.81601621996747 |
| C | -1.96162276276126 | 2.65132520016059 | 3.33972416963536 |
| C | -1.74853633849108 | 1.33110491772867 | 3.73559485535582 |
| C | -0.73347557407207 | 1.02929637109240 | 4.65004182968129 |
| C | 0.08057744054315 | 2.04279965132377 | 5.15745547291908 |
| C | -0.12898446702260 | 3.37170846627270 | 4.77225224911345 |
| C | -1.12209929047248 | 3.67555826867719 | 3.84412077212599 |
| H | -6.18248049432271 | 9.83704266533642 | 2.03084460665593 |
| H | -8.58616148586009 | 10.27898709294960 | 2.55691991522898 |
| H | -9.64377134961064 | 9.18456853196553 | 4.53688368474956 |
| H | -8.29727668762133 | 7.63524778566209 | 5.96954727516385 |
| H | -2.39832803466850 | 0.55307746399700 | 3.33422307142546 |
| H | -0.57306248234145 | -0.00670907584610 | 4.95215476132658 |
| H | 0.86416637885990 | 1.81185767564107 | 5.88002865026266 |
| H | 0.49112643854638 | 4.17866005241877 | 5.16399267146385 |

Table S31. Cartesian coordinates (in Å) of $\mathbf{1}_2 \cdot Cl^-$

| Atom | x | y | z |
|---|---|---|---|
| Sb | -2.51262268840250 | 9.70833658130928 | 2.35415271512282 |
| Sb | 0.05614311748328 | 7.46334793590832 | 2.37044120801158 |
| O | -0.71473347056266 | 9.16547786390111 | 1.68781070829889 |
| O | -2.04826980698577 | 8.33469879401187 | 3.93780429378339 |
| O | -1.86350608014254 | 11.01932016834190 | 3.85041230046244 |
| O | -0.73423508485078 | 6.09853966427274 | 1.02324507159483 |
| O | 1.49138147982348 | 7.52996268676643 | 0.86120552844299 |
| C | -1.60364006499889 | 8.99415991010189 | 5.05476916619578 |
| C | -1.34996487820152 | 8.33103668700143 | 6.25633333077918 |
| C | -0.88315143155691 | 9.04741146863900 | 7.36390191212125 |
| C | -0.72826702336195 | 10.43119215210760 | 7.28560975521714 |
| C | -1.02622099048491 | 11.10438090315770 | 6.09884949551868 |
| C | -1.50803271200926 | 10.40645014490200 | 4.98794285914940 |
| C | 1.13370158577484 | 6.81246153978434 | -0.22810196361961 |
| C | 1.89117220815826 | 6.78315160544364 | -1.40070184246357 |
| C | 1.46809440663405 | 6.00620658865578 | -2.48436611887206 |
| C | 0.28714932026209 | 5.26650264551253 | -2.40641250524796 |
| C | -0.47924261249058 | 5.29074497333762 | -1.23605283711171 |
| C | -0.05942430457576 | 6.05382618831043 | -0.15138385402147 |
| H | -1.47770212255128 | 7.25178733386637 | 6.31710395743498 |
| H | -0.67290733032171 | 8.51696131430861 | 8.29299118002412 |
| H | -0.35988632050697 | 10.99130623019710 | 8.14659002839143 |
| H | -0.91637684951871 | 12.18625988016070 | 6.02162970076989 |
| H | 2.80825164871893 | 7.37124783481615 | -1.44544189666931 |
| H | 2.06684819669136 | 5.99207456530838 | -3.39660528736937 |
| H | -0.03896627389818 | 4.66386269199653 | -3.25489924419628 |
| H | -1.40144034202824 | 4.71475847955079 | -1.16029570551277 |
| Cl | -3.40271607633195 | 7.56298009469738 | 1.01363598635961 |
| Sb | -4.02025902984076 | 6.79986877772720 | 4.59673429447498 |
| Sb | -3.04093834444961 | 5.03662072962144 | 1.84423977186890 |
| O | -4.44719977741176 | 5.46089256914876 | 3.19022085828963 |
| O | -4.54742268316505 | 8.56836359294569 | 3.64849917480846 |
| O | -6.04385786217442 | 6.91229219265041 | 5.07863428827675 |
| O | -1.73418359521637 | 5.86238640486191 | 3.33296822023259 |
| O | -2.31241909485492 | 3.29791007715532 | 2.75269180079363 |
| C | -5.87973323860626 | 8.81489685395729 | 3.67773677454485 |
| C | -6.46567530174577 | 9.88653329279277 | 3.01186067075853 |
| C | -7.84478953930611 | 10.09854235623970 | 3.11556440861728 |
| C | -8.62911665357817 | 9.23701263394194 | 3.88403108331527 |
| C | -8.04791894643622 | 8.15140910570268 | 4.54785344999557 |

| | | | |
|---|---|---|---|
| C | -6.67221196666831 | 7.93290405118770 | 4.45174715036587 |
| C | -1.43821257801169 | 3.53179883949130 | 3.74125031802407 |
| C | -0.85243792142940 | 2.50433174119432 | 4.48582171077974 |
| C | 0.10140612442325 | 2.79165335729292 | 5.46469517321800 |
| C | 0.45915054657615 | 4.11375836121750 | 5.72734272666034 |
| C | -0.12854713352758 | 5.15596929147203 | 5.00184260637025 |
| C | -1.11602801641686 | 4.87543500064241 | 4.05617914344937 |
| H | -5.84127103933441 | 10.55423068930030 | 2.41826283588062 |
| H | -8.30326011508360 | 10.94228688572980 | 2.59839830106685 |
| H | -9.70549531416618 | 9.39760801248117 | 3.96463162915117 |
| H | -8.64542886787082 | 7.46503252561386 | 5.14846880271364 |
| H | -1.13982814071336 | 1.47646201774161 | 4.26346924898283 |
| H | 0.55478117723120 | 1.97768939926240 | 6.03266351741352 |
| H | 1.21855867247518 | 4.34536351771893 | 6.47466260116149 |
| H | 0.15340313953681 | 6.18840079654041 | 5.20086149619145 |

Table S32. Cartesian coordinates (in Å) of $\mathbf{1}_2 \cdot Br^-$

| Atom | x | y | z |
|---|---|---|---|
| Sb | -2.50623906362352 | 9.70634083138303 | 2.37004277860904 |
| Sb | 0.06512741562979 | 7.46371287543502 | 2.41039418100032 |
| O | -0.70867711770518 | 9.15885164078636 | 1.71693241726757 |
| O | -2.03458717889101 | 8.32705840603989 | 3.95265977772802 |
| O | -1.87386315038054 | 11.01669251209980 | 3.88370766516886 |
| O | -0.76139667905130 | 6.14129764055697 | 1.04733547074506 |
| O | 1.49954638006129 | 7.51858954634121 | 0.90155047289923 |
| C | -1.60788410153626 | 8.98620301499940 | 5.07775341812394 |
| C | -1.36455641793020 | 8.31975181742554 | 6.27981419192980 |
| C | -0.91309512744603 | 9.03327817837158 | 7.39555234771389 |
| C | -0.76474670052444 | 10.41810449396740 | 7.32466424088441 |
| C | -1.05517919485548 | 11.09440773455170 | 6.13810216246248 |
| C | -1.52452748571844 | 10.39950210773100 | 5.01951375065557 |
| C | 1.12327836531575 | 6.82376318482858 | -0.19672095932797 |
| C | 1.88123794954018 | 6.78840871870416 | -1.36888806572621 |
| C | 1.43932223613005 | 6.03502668662107 | -2.46136496653261 |
| C | 0.24350047328532 | 5.31890747342171 | -2.39010945733553 |
| C | -0.52147970608823 | 5.34758592502756 | -1.21918517800129 |
| C | -0.08446569947395 | 6.08887189230509 | -0.12676099206894 |
| H | -1.48721876726225 | 7.23981691395644 | 6.33588001684788 |
| H | -0.70991211040007 | 8.49938970091080 | 8.32422734039075 |
| H | -0.40775176022758 | 10.97638829385560 | 8.19163211514746 |
| H | -0.95134067315953 | 12.17730020493850 | 6.06694350361619 |
| H | 2.81066845527605 | 7.35713011604269 | -1.40788135170962 |
| H | 2.03748899463393 | 6.01731762282710 | -3.37388771854449 |
| H | -0.09749726424059 | 4.73455880588305 | -3.24545122985736 |
| H | -1.45590039939303 | 4.79127493792967 | -1.14913689545486 |
| Br | -3.55650437502108 | 7.61391903819896 | 0.72504250804362 |
| Sb | -3.99570283227249 | 6.77648740528863 | 4.60506630038858 |
| Sb | -3.02553426264009 | 5.03252136010464 | 1.83747599864847 |
| O | -4.42704040681915 | 5.45326636733206 | 3.18511061797624 |
| O | -4.51423524673589 | 8.51865367554715 | 3.61267768112473 |
| O | -6.01942683064622 | 6.90288459102609 | 5.08030056114584 |
| O | -1.73484900669189 | 5.86733973966575 | 3.34463013666565 |
| O | -2.27238830164291 | 3.29527053293975 | 2.74419490607749 |
| C | -5.84569903991214 | 8.77525343082931 | 3.64004391230474 |
| C | -6.42568773147174 | 9.83512213344953 | 2.95151977017786 |
| C | -7.80370548618215 | 10.05579428453260 | 3.04896206762318 |
| C | -8.59301430941438 | 9.21213218653586 | 3.83204806122242 |
| C | -8.01736413670606 | 8.13947502111420 | 4.52087663827646 |

| | | | |
|---|---|---|---|
| C | -6.64291397124626 | 7.91123610072897 | 4.42844737212619 |
| C | -1.40912499728735 | 3.53671880447386 | 3.73888624758768 |
| C | -0.81601757663071 | 2.51257939235220 | 4.48304196036414 |
| C | 0.12903792475869 | 2.80563685825631 | 5.46821920721881 |
| C | 0.46933374815141 | 4.13047477297089 | 5.73991171571887 |
| C | -0.12807592263662 | 5.16900555971025 | 5.01710919910590 |
| C | -1.10906045852281 | 4.88228527847918 | 4.06623922317230 |
| H | -5.79751719610783 | 10.48787777922730 | 2.34576098172950 |
| H | -8.25782934649795 | 10.88959162589110 | 2.51229780360374 |
| H | -9.66865869951753 | 9.37944338167503 | 3.90841962320289 |
| H | -8.61875479118306 | 7.46790081131232 | 5.13417493949292 |
| H | -1.08948987662763 | 1.48259588285805 | 4.25305522470300 |
| H | 0.58924216900076 | 1.99424754762938 | 6.03440549620337 |
| H | 1.22218198025005 | 4.36791082062491 | 6.49198061702595 |
| H | 0.14144730828841 | 6.20294434030404 | 5.22428219243776 |

Table S33. Cartesian coordinates (in Å) of $\mathbf{1}_2 \cdot I^-$

| Atom | x | y | z |
|---|---|---|---|
| Sb | -1.06142026049727 | 5.33967017049435 | 4.27034902105256 |
| Sb | 0.27071385125887 | 5.02826532498322 | 1.17920537730077 |
| O | -1.05345416173996 | 5.88670448785293 | 2.33786869725310 |
| O | 0.16829050887931 | 6.89400720446923 | 4.77027408695854 |
| O | -2.52767131526237 | 6.77754898960217 | 4.55327457631350 |
| O | -0.30652469925389 | 6.23292796080206 | -0.38585024378932 |
| O | 1.72666920789398 | 6.42286863262594 | 1.38581310266675 |
| C | -0.54012860530063 | 8.05163939190894 | 4.88702347770413 |
| C | 0.08182526853310 | 9.26782206005634 | 5.16571660490106 |
| C | -0.68485910711687 | 10.42703259858540 | 5.32563552373227 |
| C | -2.07541494069834 | 10.36754893476210 | 5.21712499847261 |
| C | -2.70905641689501 | 9.14992747348958 | 4.94800274218761 |
| C | -1.95410015102871 | 7.98919477688138 | 4.77298888475150 |
| C | 1.50057320689515 | 7.47620873870932 | 0.55046823123022 |
| C | 2.32332083924319 | 8.60017196994697 | 0.54311858854184 |
| C | 2.07907547989321 | 9.63976854124398 | -0.36055781179024 |
| C | 1.02895450028925 | 9.54065735475501 | -1.27504598604041 |
| C | 0.20358016152961 | 8.41171451137633 | -1.28200007860079 |
| C | 0.44017471464975 | 7.37026760848291 | -0.38493561277160 |
| H | 1.16929776700248 | 9.29128261992968 | 5.24171204341048 |
| H | -0.18804491456271 | 11.37616868279230 | 5.53254230600770 |
| H | -2.67586443282238 | 11.26995208661190 | 5.34394240260089 |
| H | -3.79415607571463 | 9.08489775273922 | 4.86028769658885 |
| H | 3.13356484146424 | 8.65748726596970 | 1.27031077045926 |
| H | 2.72212393220667 | 10.52105737709900 | -0.35294896729329 |
| H | 0.83324390154882 | 10.35248386022970 | -1.97736719650832 |
| H | -0.62386216557003 | 8.31743167995782 | -1.98576626698901 |
| I | 1.84594748752208 | 4.19161855965951 | 3.79398299076927 |
| Sb | 1.23138065264829 | 1.61756959573608 | 5.54976052333204 |
| Sb | 0.72355835367437 | 1.76365378103488 | 2.19999594975492 |
| O | 0.70130777033109 | 0.69075989133313 | 3.86928920569043 |
| O | -0.36344953410151 | 2.80594052228673 | 5.83344871863412 |
| O | 0.10493488881662 | 0.32330346523533 | 6.67726751796272 |
| O | -0.82167876483582 | 0.72304170215368 | 1.32260358360583 |
| O | -0.84314047920150 | 2.91966109106952 | 2.84027743934277 |
| C | -1.38852211938926 | 2.14419713707619 | 6.43577046872876 |
| C | -2.63336965486738 | 2.73211490459585 | 6.63430479915862 |
| C | -3.63232354058540 | 2.02984414672727 | 7.31252528513052 |
| C | -3.38073998391651 | 0.73961423709818 | 7.78287209717930 |
| C | -2.14000917675409 | 0.13152567146508 | 7.56546264065628 |

| | | | |
|---|---|---|---|
| C | -1.13721571503035 | 0.83123667153655 | 6.89485680503891 |
| C | -2.01421012740668 | 2.55067813599616 | 2.24262333814546 |
| C | -3.16886142904920 | 3.31344185390764 | 2.37760887158831 |
| C | -4.35820984986944 | 2.85809850461730 | 1.80852364780484 |
| C | -4.37928705209823 | 1.65354253822415 | 1.10303083509525 |
| C | -3.20752163260204 | 0.90769616687614 | 0.93159345441196 |
| C | -2.00983809858708 | 1.36015925998362 | 1.48560561948473 |
| H | -2.80845824088284 | 3.72628021298976 | 6.22714038914747 |
| H | -4.60365625252143 | 2.49841220863990 | 7.47313884531178 |
| H | -4.16050727003569 | 0.18725626748197 | 8.30900098399573 |
| H | -1.93313613180863 | -0.88009154884483 | 7.91523280213525 |
| H | -3.10787289430708 | 4.26501144389415 | 2.89738099052389 |
| H | -5.26371697143952 | 3.45429920332940 | 1.92140264096499 |
| H | -5.30949171459162 | 1.29724744424693 | 0.65836323596152 |
| H | -3.20706345393598 | -0.02262112470802 | 0.36334935209363 |

Table S34. Cartesian coordinates (in Å) of **1**·$F_t^-$

| Atom | x | y | z |
|---|---|---|---|
| H | -4.69823501817761 | 8.42362653286035 | -0.35918311679028 |
| H | -6.41921096712511 | 7.53099407091777 | 1.22184262549339 |
| H | 5.33065829900780 | 8.39980953775385 | 1.26324542430874 |
| C | -4.40990266167749 | 8.02130125262806 | 0.61291111931438 |
| H | 5.71589097585755 | 10.78718586422650 | 1.89020393045607 |
| C | -5.36288144129675 | 7.50128706032774 | 1.49606028562557 |
| O | -2.08020117890941 | 8.39089202003830 | 0.10187890523135 |
| C | 4.54360842562438 | 8.97531417979028 | 1.75307726398227 |
| C | -3.05184692966148 | 7.99304698682117 | 0.94418356007828 |
| C | 4.75171095399427 | 10.31406100871930 | 2.08616923419844 |
| H | 3.13604812578802 | 7.32276594292986 | 1.78773218688572 |
| C | 3.30237342551797 | 8.37973331185922 | 2.00396895490732 |
| C | -4.97235180795214 | 6.99022044908123 | 2.73492267891902 |
| C | 3.73339384082597 | 11.04655504565320 | 2.70280009742334 |
| H | 3.87807939442314 | 12.09385360516050 | 2.97038566234355 |
| H | -5.71473387352008 | 6.58281334879577 | 3.42332660303165 |
| Sb | -0.22754476533812 | 8.47062942045577 | 1.12074530184367 |
| C | -2.66004674364949 | 7.49008592088372 | 2.21630813136644 |
| C | 2.29406638661861 | 9.08913983614237 | 2.66404230027293 |
| C | -3.61565912041201 | 6.96350958498626 | 3.08246323305978 |
| C | 2.48892891465699 | 10.46591810314760 | 2.96219736752759 |
| O | -0.69650746015158 | 10.27901881891450 | 1.77700962799154 |
| O | -1.33264347382971 | 7.45530988828349 | 2.50282241021812 |
| O | 1.11328448826631 | 8.52555256927012 | 3.02948659847162 |
| O | 1.52524704153072 | 11.16132712574980 | 3.59015247376494 |
| H | -3.28736820513086 | 6.56730796913185 | 4.04449975100642 |
| Sb | -0.31841225288356 | 10.32351879352720 | 3.73124809566978 |
| F | -0.97806437239633 | 12.20738175194380 | 3.77761929339834 |

Table S35. Cartesian coordinates (in Å) of **1**·$F_b^-$

| Atom | x | y | z |
|---|---|---|---|
| Sb | -2.06786223675606 | 8.84259510173011 | 3.18326574250234 |
| Sb | 0.07950120794262 | 6.84289118596121 | 1.76774685094219 |
| O | -0.32719008971552 | 8.71961831152616 | 2.24908460830833 |
| O | -1.44000846994722 | 8.17509204407097 | 4.99456206021700 |
| O | -1.46634111302344 | 10.66906932710910 | 4.02105770231370 |
| O | -1.13047924481974 | 6.72034965745465 | 0.14306722992869 |
| O | 1.41645149231855 | 7.52906015629263 | 0.30515277986892 |
| C | -0.83219293231490 | 9.14558409992671 | 5.72101978821042 |
| C | -0.26146980673034 | 8.89342010461613 | 6.96685512007357 |
| C | 0.34810536811080 | 9.93171570031685 | 7.68349295692095 |
| C | 0.35160075279508 | 11.22846455660300 | 7.16676531976009 |
| C | -0.22201753448234 | 11.49305624651540 | 5.91730867467598 |
| C | -0.83687406328881 | 10.46713305391530 | 5.19530869319406 |
| C | 0.78511431932695 | 7.69681971442465 | -0.87344514562345 |
| C | 1.40288254941174 | 8.25139957153290 | -1.99701342482457 |
| C | 0.71214551247129 | 8.33209291746834 | -3.21212337160997 |
| C | -0.61021844616863 | 7.89391499170252 | -3.30158919212892 |
| C | -1.24225308829863 | 7.33994938389433 | -2.18049897830235 |
| C | -0.56446499270020 | 7.25710525855720 | -0.96580535068316 |
| H | -0.27838599536114 | 7.87336963307476 | 7.35284697255252 |
| H | 0.79153220886250 | 9.72571578531159 | 8.65929436358444 |
| H | 0.83154299345514 | 12.03895835200380 | 7.71862240085919 |
| H | -0.22441216959284 | 12.49873464825530 | 5.49504477425933 |
| H | 2.43466479241147 | 8.59331543819890 | -1.90647784459384 |
| H | 1.20664214254466 | 8.76952386905522 | -4.08157557815105 |
| H | -1.14784536122176 | 7.95310124745315 | -4.24953656051679 |
| H | -2.27360606517515 | 6.98817345063937 | -2.22840511238144 |
| F | -1.95516073005406 | 6.59400319238952 | 2.78309352064381 |

Table S36. Cartesian coordinates (in Å) of **1**·$Cl_t^-$

| Atom | x | y | z |
|---|---|---|---|
| H | -5.02006997474640 | 8.27355046832982 | -0.19882453389642 |
| H | -6.45204137756543 | 7.82039308705080 | 1.80124065792778 |
| H | 5.76416526359554 | 8.65224866331721 | 1.94751636334144 |
| C | -4.57260279723105 | 8.00055302462435 | 0.75736680737787 |
| H | 5.62804348374683 | 11.10470483080660 | 2.40145281102585 |
| C | -5.36519677645475 | 7.75960078621316 | 1.88286536966728 |
| O | -2.42186661296396 | 8.11981401374155 | -0.26024542271776 |
| C | 4.80870323191989 | 9.11397157928836 | 2.20186477633459 |
| C | -3.17913577807586 | 7.93177487630423 | 0.83648938865170 |
| C | 4.73514222872979 | 10.48104049156710 | 2.47453062171374 |
| H | 3.69135424750785 | 7.25144524800614 | 2.08103963580569 |
| C | 3.65713219133936 | 8.32181581522152 | 2.28859194524831 |
| C | -4.76838006851943 | 7.41014266233646 | 3.09469377814376 |
| C | 3.50999688336603 | 11.07291467522190 | 2.80085562553511 |
| H | 3.43538877335255 | 12.13933914003020 | 3.01703163083978 |
| H | -5.38091741592672 | 7.22982812775386 | 3.97935108722728 |
| Sb | -0.41488540033115 | 8.24330293548028 | 0.00722897234971 |
| C | -2.57453791154535 | 7.53452475081220 | 2.05982910002828 |
| C | 2.43056570532580 | 8.90336406722626 | 2.60053785388499 |
| C | -3.37420621707179 | 7.33944582343956 | 3.19025382375276 |
| C | 2.35483818221249 | 10.29196215296460 | 2.89738840226795 |
| O | -0.47622817579437 | 9.90620174653712 | 1.09844958030296 |
| O | -1.22280633050990 | 7.37461431890703 | 2.07750954465200 |
| O | 1.29548752262457 | 8.16492133595667 | 2.72699504317883 |
| O | 1.16533137349964 | 10.78246390112240 | 3.29774668074019 |
| H | -2.89227072145130 | 7.03134311956515 | 4.11986013166545 |
| Cl | -0.34169023282423 | 9.63383419086176 | -2.07585766167993 |
| Sb | -0.34637543902120 | 9.34493141262081 | 2.99797617226891 |

Table S37. Cartesian coordinates (in Å) of **1**·$Cl_b^-$

| Atom | x | y | z |
|---|---|---|---|
| Sb | -2.17887179631896 | 8.74802601022142 | 3.25844072188474 |
| Sb | 0.00864977439471 | 6.70762511594813 | 1.74754580095712 |
| O | -0.46542582149567 | 8.55051484924541 | 2.28928349562455 |
| O | -1.49593920528349 | 8.14459151702765 | 5.06847044781349 |
| O | -1.51726926757408 | 10.59731443164050 | 3.99299356628801 |
| O | -1.14770021335718 | 6.64586779826256 | 0.08454424670514 |
| O | 1.37664558682484 | 7.49531099367045 | 0.36818626335853 |
| C | -0.83124571539181 | 9.13023279693543 | 5.72328759824820 |
| C | -0.20113928521617 | 8.91278036961313 | 6.94680866888524 |
| C | 0.45388817661369 | 9.96794599299682 | 7.59453168703662 |
| C | 0.45040164195449 | 11.24484774353650 | 7.02971852651479 |
| C | -0.18203189573737 | 11.47325754822550 | 5.80215290611861 |
| C | -0.84089088171265 | 10.42953585233650 | 5.14811608366431 |
| C | 0.77307952874065 | 7.71982380451521 | -0.81728586803178 |
| C | 1.41243627793135 | 8.34773735941391 | -1.88873140956562 |
| C | 0.74969698305238 | 8.49719140376814 | -3.11237698381696 |
| C | -0.56326192046557 | 8.04658804566289 | -3.26280368904062 |
| C | -1.21583196131570 | 7.41785464739893 | -2.19467880921807 |
| C | -0.56461281323803 | 7.26633632839010 | -0.97225563005332 |
| H | -0.21495793994079 | 7.90797566175696 | 7.37061580759228 |
| H | 0.94546142605344 | 9.79012486508872 | 8.55251463620293 |
| H | 0.96538795224176 | 12.06789242103840 | 7.52874262227833 |
| H | -0.19055857809195 | 12.46227185150970 | 5.34249053444710 |
| H | 2.43585049530175 | 8.69836117761439 | -1.75007437449850 |
| H | 1.25912354877204 | 8.99288643785850 | -3.94088206145534 |
| H | -1.07964161476499 | 8.16137412097056 | -4.21733281347801 |
| H | -2.23981566843736 | 7.05479071755226 | -2.28999690429073 |
| Cl | -2.42202581353932 | 5.98516713780114 | 2.92509392982895 |

Table S38. Cartesian coordinates (in Å) of **1**·$Br_t^-$

| Atom | x | y | z |
|---|---|---|---|
| H | -4.68101956276011 | 8.42400519163819 | -0.33596800277194 |
| H | -6.41128718274287 | 7.57320432995424 | 1.25761863050079 |
| H | 5.33441962459337 | 8.42959355384656 | 1.21729168486653 |
| C | -4.39623414026114 | 8.01983751949441 | 0.63621907016738 |
| H | 5.67019638642890 | 10.81726586597100 | 1.87005302471640 |
| C | -5.35457420877584 | 7.52400295813955 | 1.52682027849500 |
| O | -2.06093371553853 | 8.34162810708225 | 0.11433117314886 |
| C | 4.54146262750033 | 8.97850208442702 | 1.72742335509649 |
| C | -3.03860994567362 | 7.96844950858464 | 0.96384618661643 |
| C | 4.72120904271124 | 10.31802856480610 | 2.07411116855010 |
| H | 3.17473014662424 | 7.29174248825601 | 1.75812302285336 |
| C | 3.31986540019801 | 8.34860288510415 | 1.98904110910748 |
| C | -4.96842582774836 | 7.01072000401068 | 2.76620304646977 |
| C | 3.69613431004678 | 11.01747037029360 | 2.71673183733132 |
| H | 3.81762775409661 | 12.06406446493150 | 2.99746498608373 |
| H | -5.71587748960311 | 6.62448662492480 | 3.46103728140723 |
| Sb | -0.21213121263334 | 8.39432911479490 | 1.11888171615970 |
| C | -2.65109407161719 | 7.46220690984900 | 2.23451528394025 |
| C | 2.30390370484345 | 9.02596155738081 | 2.67040242827803 |
| C | -3.61169568846956 | 6.95963589337921 | 3.10881500033923 |
| C | 2.47157773168323 | 10.40097960333160 | 2.98668870115430 |
| O | -0.65780332933907 | 10.20505928071200 | 1.80336194927118 |
| O | -1.32110005213739 | 7.40162638198033 | 2.51445057206597 |
| O | 1.13769131435562 | 8.42642636020133 | 3.03729643318567 |
| O | 1.50380439425598 | 11.06265921992480 | 3.64915902800126 |
| H | -3.28702500387202 | 6.56197038151811 | 4.07133356487714 |
| Sb | -0.31454820960874 | 10.17095368775510 | 3.76287461663362 |
| Br | -1.37874279655686 | 12.60649708770760 | 3.97636285345474 |

Table S39. Cartesian coordinates (in Å) of **1**·$Br_b^-$

| Atom | x | y | z |
|---|---|---|---|
| Sb | -2.18516852443855 | 8.79899989181573 | 3.25140280932917 |
| Sb | -0.06546229523499 | 6.66162557566467 | 1.75392202608058 |
| O | -0.47522334174842 | 8.51785067289365 | 2.29891820660552 |
| O | -1.53069083487687 | 8.20403070258614 | 5.07414683481559 |
| O | -1.46468199948730 | 10.63755107023960 | 3.95640875180380 |
| O | -1.20919842395423 | 6.65767398155658 | 0.08150990817020 |
| O | 1.34639997527503 | 7.39897485952929 | 0.39063351885289 |
| C | -0.83918367033056 | 9.17891999188215 | 5.71736863269731 |
| C | -0.22224719253600 | 8.96130642083834 | 6.94769186167378 |
| C | 0.46043973085762 | 10.00635291251840 | 7.58272487573357 |
| C | 0.50021750394728 | 11.27350384962760 | 6.99749035347895 |
| C | -0.11798650192848 | 11.50174196705020 | 5.76276399675696 |
| C | -0.80383517373250 | 10.46790771555890 | 5.12117296095455 |
| C | 0.76217681610564 | 7.65449711747990 | -0.79913573988424 |
| C | 1.43651594278452 | 8.26073115999258 | -1.86145351434484 |
| C | 0.78983789264970 | 8.44697544295464 | -3.08852721887142 |
| C | -0.54010954958013 | 8.05401041458354 | -3.25152142475032 |
| C | -1.22745407434695 | 7.44753939367242 | -2.19264989256520 |
| C | -0.59217667427324 | 7.25987626759993 | -0.96676317228744 |
| H | -0.27020102245318 | 7.96439684751559 | 7.38722888420646 |
| H | 0.94131629105811 | 9.82890592649648 | 8.54616183322958 |
| H | 1.03689558400819 | 12.08816656061550 | 7.48724149905663 |
| H | -0.09275712253137 | 12.48278763293420 | 5.28702580016404 |
| H | 2.47284642922552 | 8.56635258463536 | -1.71278671459225 |
| H | 1.32611826655115 | 8.92538718124983 | -3.91016226381782 |
| H | -1.04390587866718 | 8.19766096298725 | -4.20883802307508 |
| H | -2.26522686637855 | 7.12913989111673 | -2.29768691001640 |
| Br | -2.64785428596423 | 5.89136000440444 | 2.97283112059547 |

Table S40. Cartesian coordinates (in Å) of **1**·$I_t^-$

| Atom | x | y | z |
|---|---|---|---|
| H | -4.14227042563543 | 8.44637343086126 | -0.49188344295744 |
| H | -6.08318661094712 | 8.13641314055908 | 1.05406900039596 |
| H | 4.69039255299764 | 8.70284019606529 | 0.52592823364588 |
| C | -3.98517675981019 | 8.16696877805355 | 0.55069155313107 |
| H | 4.67937465387279 | 11.14913865641120 | 0.99248887428603 |
| C | -5.06414687453383 | 8.00834616878084 | 1.42444662807841 |
| O | -1.64661460309884 | 8.16300496134101 | 0.11834527532944 |
| C | 4.10532487348448 | 9.10489230046653 | 1.35266157487286 |
| C | -2.66635554958730 | 8.01659085082716 | 0.99380801778144 |
| C | 4.02356955874010 | 10.48114955553530 | 1.55271873188838 |
| H | 3.26138602365387 | 7.17056136214179 | 1.87999297993626 |
| C | 3.25018251440400 | 8.24758153603969 | 2.05383121944669 |
| C | -4.83600445181201 | 7.65091738160418 | 2.75337343810339 |
| C | 3.18971993460179 | 11.00746239224220 | 2.54477669859779 |
| H | 3.08594253283474 | 12.08485639440900 | 2.67414411652849 |
| H | -5.67051190463759 | 7.53421523614320 | 3.44689037340188 |
| Sb | 0.22499310190232 | 8.11946065500326 | 0.95707387179384 |
| C | -2.43334274182143 | 7.60950096124677 | 2.34280124857204 |
| C | 2.36647885443615 | 8.76929615294894 | 2.99786504854724 |
| C | -3.52415333833775 | 7.49044798841782 | 3.21202226955147 |
| C | 2.30820651160531 | 10.17069351039790 | 3.22808832625428 |
| O | -0.26407960417525 | 9.80487815062464 | 1.96097022132417 |
| O | -1.16113466065463 | 7.34581456796532 | 2.74842908574826 |
| O | 1.39515807168001 | 7.99409324197910 | 3.58631613327351 |
| O | 1.35463398970806 | 10.61558973880380 | 4.07687164523326 |
| H | -3.32647302403038 | 7.18458074499103 | 4.24143544550807 |
| I | 1.39596641906953 | 9.88876815177161 | -0.87301075198157 |
| Sb | -0.23218904390905 | 9.24090379436830 | 3.84943418370890 |

Table S41. Cartesian coordinates (in Å) of **1**·$I_b^-$

| Atom | x | y | z |
|---|---|---|---|
| Sb | -2.09707565662945 | 8.94727812808116 | 3.14252816029529 |
| Sb | 0.08238543384953 | 6.79731671311280 | 1.78928191399760 |
| O | -0.34729315752968 | 8.67202846485528 | 2.25836023772877 |
| O | -1.49446389577037 | 8.25296303613585 | 4.96402378430972 |
| O | -1.39774970666950 | 10.74551112851640 | 3.96939934114874 |
| O | -1.14330240459684 | 6.72941013131089 | 0.15984304800202 |
| O | 1.43208917605613 | 7.47157131369969 | 0.32978843149779 |
| C | -0.83658862017215 | 9.19888368561169 | 5.67838786406325 |
| C | -0.26793352459562 | 8.92519489200304 | 6.92154099206170 |
| C | 0.38970731997650 | 9.93776606013388 | 7.63091091747197 |
| C | 0.44909523896696 | 11.23174056040120 | 7.10960289555750 |
| C | -0.12163078787350 | 11.51733897707920 | 5.86422909214505 |
| C | -0.78284613092475 | 10.51679491051930 | 5.14828243446568 |
| C | 0.79797222036331 | 7.67222328007386 | -0.84403094820646 |
| C | 1.42757871586528 | 8.22967267610814 | -1.95922463375228 |
| C | 0.73359991526531 | 8.36081132591934 | -3.16728564408272 |
| C | -0.60223199570689 | 7.96458694332501 | -3.25820685115034 |
| C | -1.24573761721262 | 7.40712699512796 | -2.14634669815525 |
| C | -0.56402558321541 | 7.27585148121937 | -0.93731639912958 |
| H | -0.32956299305270 | 7.90819397098137 | 7.31077573872890 |
| H | 0.83238387837747 | 9.71415401594332 | 8.60311482487176 |
| H | 0.96572920674865 | 12.02192817522910 | 7.65762654233571 |
| H | -0.07974272704928 | 12.52032956195690 | 5.43774620836801 |
| H | 2.46926529301961 | 8.53962080655841 | -1.86717683934997 |
| H | 1.23655090775075 | 8.80062918590441 | -4.03058084141829 |
| H | -1.14391526102043 | 8.06383017462509 | -4.20040879446613 |
| H | -2.28744875957894 | 7.08773323544944 | -2.19496431032575 |
| I | -2.59540748464132 | 5.95373717011771 | 2.95721853298734 |

Table S42. Cartesian coordinates (in Å) of **1**·2$F_b^-$

| Atom | x | y | z |
|---|---|---|---|
| Sb | -2.47275847571124 | 7.24806880159920 | 4.43857987900707 |
| Sb | -1.42025817481277 | 5.86047509038695 | 1.57625732372872 |
| O | -2.09132061104842 | 7.48366137308595 | 2.53954046470775 |
| O | -0.59629149801567 | 7.55456979211249 | 5.23205410086323 |
| O | -2.43071054056784 | 9.44884505532536 | 4.70083505962970 |
| O | -1.80997879984250 | 6.74628160994713 | -0.27099837582852 |
| O | 0.47656545548087 | 6.96732104141323 | 1.14110637985646 |
| C | -0.25992546695703 | 8.84018181698863 | 5.42086598934626 |
| C | 0.98847986000411 | 9.21216345601043 | 5.91991903564693 |
| C | 1.29449285421617 | 10.56039312637670 | 6.16854981412419 |
| C | 0.35100925852744 | 11.54667481952430 | 5.87802036290312 |
| C | -0.91262782990779 | 11.18933997348300 | 5.38458183722578 |
| C | -1.24218392565865 | 9.84714184599798 | 5.13713669607120 |
| C | 0.40303863384263 | 7.61010525787331 | -0.01038547554318 |
| C | 1.43280065701589 | 8.41213397960977 | -0.53383646060592 |
| C | 1.31922619327980 | 9.01521041507636 | -1.79636288233603 |
| C | 0.13927597466374 | 8.88682130019502 | -2.53084499453157 |
| C | -0.91028334837675 | 8.10107622613053 | -2.02375811191287 |
| C | -0.81040822772909 | 7.48338570463010 | -0.77508781943710 |
| H | 1.71695334984803 | 8.42402749191658 | 6.12131509345445 |
| H | 2.28876052803535 | 10.83259647231650 | 6.53275491426641 |
| H | 0.57713773481198 | 12.60036834380280 | 6.06670460270841 |
| H | -1.66147011133372 | 11.94989611947540 | 5.15172539434205 |
| H | 2.34358850654206 | 8.52034528211884 | 0.05957170784101 |
| H | 2.13665204621417 | 9.63926832097036 | -2.17052470073675 |
| H | 0.04638795696309 | 9.34522487826321 | -3.51968173624990 |
| H | -1.84307688154782 | 7.98152613536149 | -2.58046234339317 |
| F | -1.72108264941324 | 5.28747981499232 | 4.30389855345294 |
| F | -3.39379046852281 | 5.27450545501575 | 1.36487269139932 |

Table S43. Cartesian coordinates (in Å) of **1**·$F_b^-F_t^-$

| Atom | x | y | z |
|---|---|---|---|
| Sb | -2.76870198473958 | 9.24477008455146 | 3.28752143689115 |
| Sb | -0.55860425036601 | 7.22823966198291 | 1.94104837614839 |
| O | -1.14199406331366 | 9.08988649317759 | 2.13871756521385 |
| O | -1.51327837871947 | 8.21198127659726 | 4.87496095833128 |
| O | -1.94552869491091 | 10.83308355451280 | 4.37142554112969 |
| O | -1.37414855138477 | 6.87556661604087 | 0.06764079595594 |
| O | 1.03939171514219 | 7.95750959114810 | 0.58835295821679 |
| C | -0.79147817687840 | 9.09770465247104 | 5.54097106531949 |
| C | 0.13689540002832 | 8.75737994136354 | 6.54050840463008 |
| C | 0.84239184875679 | 9.73968689763480 | 7.25351485001923 |
| C | 0.58823610842670 | 11.09108153313870 | 7.01615151219937 |
| C | -0.32847602692433 | 11.45925821265410 | 6.01655366737509 |
| C | -1.02892928035907 | 10.49512792935300 | 5.28661314858775 |
| C | 0.66725766617807 | 7.85587354154750 | -0.68025790863845 |
| C | 1.46269970769493 | 8.27461825386390 | -1.75939197913223 |
| C | 1.04523901295925 | 8.08696369644631 | -3.08602389233593 |
| C | -0.20635826451834 | 7.53133320515413 | -3.35415228717937 |
| C | -1.02189353673392 | 7.11127069684261 | -2.28953626165333 |
| C | -0.61531661723730 | 7.27267009431977 | -0.96380982064609 |
| H | 0.31673642837806 | 7.69530608871718 | 6.72507004896450 |
| H | 1.54835687074650 | 9.43903450596073 | 8.03375336466707 |
| H | 1.14402783774030 | 11.86462342134810 | 7.55381970907200 |
| H | -0.53020066269549 | 12.51063472874520 | 5.79763553968346 |
| H | 2.43340038020776 | 8.72167820404490 | -1.53260219845144 |
| H | 1.68361155293807 | 8.43145695698742 | -3.90508419747794 |
| H | -0.53736257963810 | 7.37840265748088 | -4.38510712650928 |
| H | -2.00237227412443 | 6.66705355152001 | -2.47526865801424 |
| F | -2.52091106579582 | 6.65693137011229 | 2.50295165938013 |
| F | -3.40694912085734 | 10.76708258228260 | 2.04783272825302 |

Table S44. Cartesian coordinates (in Å) of **1**·2$F_t^-$

| Atom | x | y | z |
|---|---|---|---|
| H | -4.89700739477017 | 8.27190072530789 | -0.36700349387370 |
| H | -6.59436067653351 | 7.70864373479318 | 1.38959929664834 |
| H | 5.73616533005663 | 8.73960049474899 | 1.43210897406764 |
| C | -4.58068104551095 | 7.97077141939178 | 0.63454403499463 |
| H | 5.76735393872165 | 11.13346522407260 | 2.17420997711593 |
| C | -5.52744618160610 | 7.67913927548526 | 1.62920163667299 |
| O | -2.30098926824906 | 8.17819321046590 | -0.04877665206049 |
| C | 4.84641797407414 | 9.19528724587335 | 1.87632349664389 |
| C | -3.20738768468424 | 7.93385680678403 | 0.90248003391010 |
| C | 4.85372343723349 | 10.53763081206510 | 2.25644888914110 |
| H | 3.64785164326246 | 7.38802582419371 | 1.70532151383809 |
| C | 3.66949718515640 | 8.44087214321724 | 1.99634188589145 |
| C | -5.09670040492809 | 7.29308925929201 | 2.89876970898355 |
| C | 3.69479702250585 | 11.10904030513010 | 2.80505643367661 |
| H | 3.67952270433339 | 12.15731624326980 | 3.11255731816614 |
| H | -5.82184060002220 | 7.07836139427869 | 3.68917218767901 |
| Sb | -0.30324153293014 | 8.20878426672295 | 0.58933689715747 |
| C | -2.76008909238335 | 7.51430777946664 | 2.20331850255275 |
| C | 2.50619206304193 | 8.98409773158211 | 2.56407749894937 |
| C | -3.72438994636313 | 7.24894071446961 | 3.18808470194406 |
| C | 2.51038909181021 | 10.37425567592650 | 2.93216196379899 |
| O | -0.54178859589392 | 9.95574411253706 | 1.50277385993078 |
| O | -1.45124358629565 | 7.37099423676051 | 2.40392420285337 |
| O | 1.40725027503132 | 8.27099456806136 | 2.80310310124499 |
| O | 1.41366721172932 | 10.90424992150250 | 3.48336063279815 |
| H | -3.37047799904482 | 6.94712641697888 | 4.17668498356317 |
| F | -0.01809548851541 | 9.25197658920363 | -1.16083958499817 |
| Sb | -0.29230942313719 | 9.68717709824415 | 3.45543213480436 |
| F | -1.27519195608886 | 11.47029477017410 | 3.74352886390543 |

Table S45. Cartesian coordinates (in Å) of **1**·2$Cl_b^-$

| Atom | x | y | z |
|---|---|---|---|
| Sb | -1.81654453182369 | 7.00747307462925 | 4.43204219475154 |
| Sb | -1.62890267540490 | 6.06919057519211 | 1.30969468381816 |
| O | -1.11771258877813 | 7.44976057562999 | 2.63257024764287 |
| O | -0.01141348102102 | 7.66818271187892 | 5.30583127603435 |
| O | -2.28428867792715 | 9.03889370951369 | 4.76503735356655 |
| O | -1.98012655122660 | 7.56765208426968 | -0.13577769907623 |
| O | 0.28141069407763 | 6.18379684560677 | 0.41981920597832 |
| C | -0.06305672602979 | 8.96733213211662 | 5.62729445410061 |
| C | 1.00106577178901 | 9.63164005242012 | 6.24745555689219 |
| C | 0.91457876349363 | 10.99683595044390 | 6.56166393916015 |
| C | -0.26010955333120 | 11.70040544747120 | 6.29233008330452 |
| C | -1.33203951148154 | 11.05468647658050 | 5.65657618705898 |
| C | -1.26678931891032 | 9.69322519228344 | 5.34049077033321 |
| C | 0.31381065886288 | 7.08877206147849 | -0.56750716695289 |
| C | 1.47214686811111 | 7.35200308788778 | -1.30678019621390 |
| C | 1.46144150493366 | 8.28088402735004 | -2.35897609520550 |
| C | 0.29937456051238 | 9.00120805765049 | -2.63883551474593 |
| C | -0.87128599838341 | 8.75507234634813 | -1.90462245426432 |
| C | -0.88364076536697 | 7.82166398957609 | -0.86208472632792 |
| H | 1.91066801723543 | 9.06223028483583 | 6.44927721513447 |
| H | 1.75344863393622 | 11.49071058987270 | 7.05970508792608 |
| H | -0.32943947293370 | 12.76808923584370 | 6.51766208962430 |
| H | -2.25354318211866 | 11.59005267801660 | 5.41889768426814 |
| H | 2.37499632299986 | 6.79086002621442 | -1.05727143147862 |
| H | 2.38237544379490 | 8.47900092260372 | -2.91413833994359 |
| H | 0.28068980827522 | 9.72437477537433 | -3.45882911522427 |
| H | -1.79122266426749 | 9.30766260985881 | -2.10647638505428 |
| Cl | -0.48356462518564 | 4.55981380875557 | 3.53492744973771 |
| Cl | -4.13412472383175 | 6.76761567029683 | 2.66637064515528 |

Table S46. Cartesian coordinates (in Å) of **1**·$Cl_b^-Cl_t^-$

| Atom | x | y | z |
|---|---|---|---|
| Sb | -3.43389653797828 | 9.22111705055382 | 3.62279082971437 |
| Sb | -1.23722763958142 | 7.20028293128506 | 2.32509940482975 |
| O | -2.20011350863559 | 8.93317341302451 | 2.11182886862991 |
| O | -1.81910524284713 | 8.10711331775559 | 4.78420846816684 |
| O | -2.27646631535812 | 10.75494473615720 | 4.40995576719071 |
| O | -1.54560638785437 | 6.77901592240494 | 0.29273780452081 |
| O | 0.47853132644111 | 8.17147055613288 | 1.44326131878767 |
| C | -0.83638138834449 | 8.97279842240179 | 5.07886259726628 |
| C | 0.41959585514912 | 8.57170289980477 | 5.55061914661735 |
| C | 1.36622208394310 | 9.51423601376453 | 5.97662581899613 |
| C | 1.09697223802872 | 10.87676530715000 | 5.84391392454565 |
| C | -0.13431871862778 | 11.29623778398850 | 5.32124195196826 |
| C | -1.08737486159948 | 10.36809483326500 | 4.88957158347595 |
| C | 0.46446339625863 | 8.06147967236322 | 0.11381877440150 |
| C | 1.44383650651008 | 8.63373726205365 | -0.71007890387863 |
| C | 1.42304999379076 | 8.44311121224068 | -2.10001963361675 |
| C | 0.38158989147786 | 7.72568327816037 | -2.69054552003578 |
| C | -0.61249607266241 | 7.14809968603950 | -1.88465850542277 |
| C | -0.60011413376960 | 7.31672606862647 | -0.49656914728876 |
| H | 0.59816964303365 | 7.50055752501178 | 5.66470415790161 |
| H | 2.33544985094277 | 9.17430559556307 | 6.35068181212013 |
| H | 1.82959730288110 | 11.61992585219820 | 6.17018121286286 |
| H | -0.35853307663785 | 12.35756070506920 | 5.19615802678208 |
| H | 2.24041804261731 | 9.20662213327382 | -0.23065904042270 |
| H | 2.19311102037859 | 8.91020087243384 | -2.72054803917550 |
| H | 0.36086411147301 | 7.56797406454266 | -3.77236851814302 |
| H | -1.43730548907659 | 6.58255621137023 | -2.32346817075671 |
| Cl | -3.76572761390114 | 6.22672890302995 | 2.66477968854232 |
| Cl | -4.67146327605160 | 11.10398777033440 | 2.27168332142040 |

Table S47. Cartesian coordinates (in Å) of **1**·2$Cl_t^-$

| Atom | x | y | z |
|---|---|---|---|
| H | -4.81687631859428 | 8.23001755938764 | -0.35950092188076 |
| H | -6.52765126972589 | 7.72979266959458 | 1.40204508379860 |
| H | 5.67236031340661 | 8.73634355650060 | 1.36532578247346 |
| C | -4.51073760958812 | 7.95200486866284 | 0.65111848666898 |
| H | 5.70218478565940 | 11.11030128723180 | 2.16552369062554 |
| C | -5.46257096442403 | 7.69299115641505 | 1.64694418889266 |
| O | -2.22614450987979 | 8.12276748834664 | -0.02532463882111 |
| C | 4.78755252558923 | 9.17600741696970 | 1.83311821788631 |
| C | -3.13957800725575 | 7.91155890987468 | 0.93107630479793 |
| C | 4.79303214162447 | 10.50830086802780 | 2.24730453970756 |
| H | 3.59215015952962 | 7.37111463639347 | 1.62878556733649 |
| C | 3.61547176560967 | 8.41530483441418 | 1.94767634426166 |
| C | -5.04384487594240 | 7.33860888387191 | 2.92979194524364 |
| C | 3.64086078322976 | 11.06319222593810 | 2.82112295454224 |
| H | 3.62408147082275 | 12.10323096764260 | 3.15320502782581 |
| H | -5.77500365112869 | 7.15388000130181 | 3.72123078388497 |
| Sb | -0.24791318767630 | 8.14840419446255 | 0.64809376678462 |
| C | -2.70846356367171 | 7.52131322453814 | 2.24066263036614 |
| C | 2.46290886850837 | 8.94282703305923 | 2.54333243919450 |
| C | -3.67481769273266 | 7.29269531186190 | 3.22825427565322 |
| C | 2.46125804722113 | 10.31891524830670 | 2.94271054826848 |
| O | -0.53475778806807 | 9.91085642714006 | 1.52492220602337 |
| O | -1.39185342060480 | 7.36999483057550 | 2.46136952098664 |
| O | 1.36287193603048 | 8.20794223628734 | 2.77763341864762 |
| O | 1.36920286836857 | 10.83326744294980 | 3.52275205863040 |
| H | -3.32817141765571 | 7.01773226026391 | 4.22668023733151 |
| Cl | 0.28855306250417 | 9.46265101625783 | -1.54785820623004 |
| Sb | -0.31116659396857 | 9.59203068903070 | 3.47574193273766 |
| Cl | -1.70335085718748 | 11.77009075469260 | 3.86756481436191 |

Table S48. Cartesian coordinates (in Å) of **1**·2$Br_b^-$

| Atom | x | y | z |
|---|---|---|---|
| Sb | -1.82492644659716 | 6.99274358749397 | 4.44165805179364 |
| Sb | -1.58399140214338 | 6.02439135390794 | 1.29898208135533 |
| O | -1.11751698284412 | 7.40638690682207 | 2.63884171426588 |
| O | -0.03682505503981 | 7.67785197500833 | 5.31644821891615 |
| O | -2.31340288666545 | 9.01933304504939 | 4.73482909379579 |
| O | -1.94343779848070 | 7.51988170112471 | -0.13910972713954 |
| O | 0.33388216744846 | 6.18026894924733 | 0.44525303375344 |
| C | -0.09981092075777 | 8.98316747343456 | 5.61576487327685 |
| C | 0.95516058737124 | 9.66533401740224 | 6.23120298577141 |
| C | 0.85439307658663 | 11.03449452033480 | 6.52165456037571 |
| C | -0.32398070932003 | 11.72373458030470 | 6.23152488708117 |
| C | -1.38645804652302 | 11.05895420515290 | 5.60032219824140 |
| C | -1.30575225949754 | 9.69344857921950 | 5.30771394874379 |
| C | 0.36506470196234 | 7.09069985992626 | -0.53872119476133 |
| C | 1.52958829274932 | 7.37874824447651 | -1.25809412643966 |
| C | 1.51638765325032 | 8.31337146753775 | -2.30476929886150 |
| C | 0.34463817675921 | 9.01204290037359 | -2.59932747091087 |
| C | -0.83211768674000 | 8.73980989135052 | -1.88493946102593 |
| C | -0.84091602158251 | 7.80027440496063 | -0.84835724987792 |
| H | 1.86764713426665 | 9.10682818860178 | 6.44898694515963 |
| H | 1.68596612718784 | 11.54430536606470 | 7.01554292500709 |
| H | -0.40399897758408 | 12.79407609725520 | 6.43935147744468 |
| H | -2.31068111423842 | 11.58197099441900 | 5.34693965687005 |
| H | 2.43894798151591 | 6.83374007489452 | -0.99736038129521 |
| H | 2.44122125458484 | 8.53175518429747 | -2.84539211111943 |
| H | 0.32491874690297 | 9.73989425656630 | -3.41495451843452 |
| H | -1.75958161305739 | 9.27500654601319 | -2.09808567486803 |
| Br | -0.34873713541735 | 4.41249663831141 | 3.61476048817200 |
| Br | -4.28747884409701 | 6.73407799044849 | 2.60568107470997 |

Table S49. Cartesian coordinates (in Å) of **1**·$Br_b^-Br_t^-$

| Atom | x | y | z |
|---|---|---|---|
| Sb | -3.44542351235606 | 9.21453197435256 | 3.64488569950056 |
| Sb | -1.25687083417696 | 7.18553614651061 | 2.34142671367564 |
| O | -2.24748036979041 | 8.90002298397647 | 2.10845886086706 |
| O | -1.83175205253234 | 8.10769841032186 | 4.78550785969043 |
| O | -2.25801949384496 | 10.75318866607150 | 4.37928824124570 |
| O | -1.54071169631767 | 6.76300789372567 | 0.31023989350416 |
| O | 0.45858805460846 | 8.15617665202981 | 1.49988053273954 |
| C | -0.83209316119666 | 8.96600505877979 | 5.05625494320322 |
| C | 0.42372856696911 | 8.55193746518216 | 5.51463776258096 |
| C | 1.39080343890206 | 9.48706436475689 | 5.90895282127411 |
| C | 1.14008418986015 | 10.85100213373220 | 5.75499822250356 |
| C | -0.09246497500470 | 11.28129581742200 | 5.24552369952320 |
| C | -1.06603665143839 | 10.35982163336670 | 4.84645978574521 |
| C | 0.45925010373172 | 8.06338238734178 | 0.16574288231918 |
| C | 1.44540228905644 | 8.65157229637160 | -0.63649802142871 |
| C | 1.43983787658873 | 8.48064037007030 | -2.02879465736394 |
| C | 0.40962267455653 | 7.76393981094877 | -2.63975599431778 |
| C | -0.59012054450205 | 7.17001373109308 | -1.85423077088794 |
| C | -0.59256520316696 | 7.32032536533808 | -0.46406732879410 |
| H | 0.58608781327858 | 7.48035508640374 | 5.64658951887840 |
| H | 2.36106666977600 | 9.13938888614346 | 6.27244549513935 |
| H | 1.88989031320208 | 11.58802941571170 | 6.05455607274592 |
| H | -0.30252138784548 | 12.34322013830060 | 5.10385310989737 |
| H | 2.23173756914689 | 9.22392460415648 | -0.14028225794352 |
| H | 2.21348715639850 | 8.96030738696026 | -2.63466488049399 |
| H | 0.39999385534608 | 7.62377175548173 | -3.72398144182261 |
| H | -1.40679055492227 | 6.60595876849057 | -2.30929154691953 |
| Br | -3.95964679062895 | 6.13186124876280 | 2.73527096459831 |
| Br | -4.81134234369746 | 11.22222954819650 | 2.21040282034022 |

Table S50. Cartesian coordinates (in Å) of **1**·2$Br_t^-$

| Atom | x | y | z |
|---|---|---|---|
| H | -4.81358517088742 | 8.22874910924514 | -0.35056868932113 |
| H | -6.51331587500090 | 7.71387645646584 | 1.41711391253704 |
| H | 5.65586284326497 | 8.70833243725331 | 1.36804839791416 |
| C | -4.50212642408412 | 7.94905072921899 | 0.65770162094801 |
| H | 5.69944906325714 | 11.07840343829440 | 2.17728627398208 |
| C | -5.44709193026443 | 7.68060090716869 | 1.65667537563840 |
| O | -2.21972239907982 | 8.13231763519318 | -0.02610931785853 |
| C | 4.77354798454352 | 9.15133721684925 | 1.83677797271607 |
| C | -3.13002334316927 | 7.91500886765229 | 0.93313719260814 |
| C | 4.78681774926191 | 10.48175615966950 | 2.25706313692461 |
| H | 3.56639363471547 | 7.35581213711340 | 1.62160463169037 |
| C | 3.59669075557928 | 8.39800980314048 | 1.94587637333216 |
| C | -5.02140601186735 | 7.32436914927533 | 2.93680300234900 |
| C | 3.63856038624453 | 11.04235273133110 | 2.83160960979090 |
| H | 3.62777764351646 | 12.08071362427670 | 3.16836653716371 |
| H | -5.74819592271400 | 7.13352879158739 | 3.73044685830588 |
| Sb | -0.24563048712269 | 8.16714067839936 | 0.64571429056898 |
| C | -2.69266268464881 | 7.52368904775746 | 2.23821512908113 |
| C | 2.44823752130385 | 8.93235166803340 | 2.54117962649700 |
| C | -3.65134959714303 | 7.28495950041134 | 3.22957189763330 |
| C | 2.45477009458971 | 10.30415405507470 | 2.94800595046952 |
| O | -0.54029200924122 | 9.92816914231804 | 1.52537988914328 |
| O | -1.37112443507275 | 7.38197975682105 | 2.45456156565502 |
| O | 1.33898528165282 | 8.20292993967378 | 2.76695857564591 |
| O | 1.36498331230801 | 10.82040594110880 | 3.53259427520000 |
| H | -3.29882084920820 | 7.00952343152141 | 4.22564733893342 |
| Br | 0.33806586368639 | 9.57422411115168 | -1.70317907066438 |
| Sb | -0.31634511373369 | 9.58828431000689 | 3.47337730410462 |
| Br | -1.80886288068638 | 11.91210722398690 | 3.93144333901131 |

Table S51. Cartesian coordinates (in Å) of **1**·2$I_b^-$

| Atom | x | y | z |
|---|---|---|---|
| Sb | -1.82988648978284 | 7.01030059436532 | 4.45902184622950 |
| Sb | -1.64886461766305 | 6.06237090472657 | 1.27011042400402 |
| O | -1.14737598949738 | 7.41744757195477 | 2.63625818430664 |
| O | -0.00420707087830 | 7.66427100137413 | 5.29515434634875 |
| O | -2.27778343780728 | 9.05334642528965 | 4.74791029269797 |
| O | -1.98186002688282 | 7.60294124660482 | -0.13632933909844 |
| O | 0.27913349132535 | 6.19796146251586 | 0.42057884757879 |
| C | -0.05385705793781 | 8.96621906764198 | 5.61070727799767 |
| C | 1.03044423102435 | 9.63771315366031 | 6.18617231331532 |
| C | 0.94147965419176 | 10.99527970229470 | 6.52958166232426 |
| C | -0.22129524181816 | 11.71021106278040 | 6.23983737146223 |
| C | -1.31645512550196 | 11.05720721256550 | 5.65425938590040 |
| C | -1.25364864862344 | 9.69895877645872 | 5.32327267619533 |
| C | 0.31522937779162 | 7.11135881050444 | -0.55979116963677 |
| C | 1.48033462707794 | 7.38293032010127 | -1.28530309986014 |
| C | 1.48294356445937 | 8.32744712545074 | -2.32297389156893 |
| C | 0.32606893452224 | 9.05633985605790 | -2.60145996403337 |
| C | -0.85010482811090 | 8.80533856563983 | -1.87864117827686 |
| C | -0.87751587393912 | 7.85275493185921 | -0.85376952533781 |
| H | 1.93757720835383 | 9.06382579644675 | 6.38592537806501 |
| H | 1.80635413506883 | 11.49960841844160 | 6.96891529205205 |
| H | -0.30136459347627 | 12.76818265919960 | 6.50380327103246 |
| H | -2.23498901082038 | 11.59799440036300 | 5.41746105850148 |
| H | 2.37944408806355 | 6.81533870262735 | -1.03711452657315 |
| H | 2.40888634734142 | 8.52870933158118 | -2.86841827547951 |
| H | 0.31709296734836 | 9.79396140217661 | -3.40853831595079 |
| H | -1.76582728523538 | 9.36528250310717 | -2.07917075955928 |
| I | -0.60647753291512 | 4.24663957335447 | 3.60463830224299 |
| I | -4.39527379567844 | 6.57914842085600 | 2.70424911512018 |

Table S52. Cartesian coordinates (in Å) of **1**·$I_b^-I_t^-$

| Atom | x | y | z |
|---|---|---|---|
| Sb | -3.42995975633388 | 9.18036408665252 | 3.68144816140853 |
| Sb | -1.22699614093719 | 7.22340403938108 | 2.32748534142507 |
| O | -2.19366548075782 | 8.95721167226558 | 2.14493290328690 |
| O | -1.78663179007865 | 8.07942307040917 | 4.78914236987645 |
| O | -2.26283652315611 | 10.74884520194560 | 4.41823407963362 |
| O | -1.56817693053262 | 6.83913950657660 | 0.29300365598376 |
| O | 0.49679550833073 | 8.16288518631800 | 1.46512874031057 |
| C | -0.81046707705733 | 8.96188500157879 | 5.06987803272203 |
| C | 0.45048869973735 | 8.56687666353643 | 5.53128721334605 |
| C | 1.40179539907328 | 9.50976140788221 | 5.94385201902104 |
| C | 1.12832227521955 | 10.87116764468850 | 5.80833652778919 |
| C | -0.10953115615627 | 11.28615868188840 | 5.30039020093734 |
| C | -1.07027467996278 | 10.35710927432260 | 4.88340808547090 |
| C | 0.48521789751615 | 8.05428093155035 | 0.13260539646955 |
| C | 1.48425140398236 | 8.60456846910752 | -0.68076126460437 |
| C | 1.46481699485896 | 8.42713901800766 | -2.07210755508246 |
| C | 0.40597646628753 | 7.74432901069438 | -2.67250775643203 |
| C | -0.60917201047324 | 7.19101304429605 | -1.87705601273300 |
| C | -0.60020535004502 | 7.35108647474949 | -0.48770843384368 |
| H | 0.63185485721769 | 7.49580794475637 | 5.64255322556487 |
| H | 2.37588938840651 | 9.17185788325760 | 6.30634543303545 |
| H | 1.86361218103533 | 11.61719457575450 | 6.12172220969418 |
| H | -0.33851140081532 | 12.34672384328920 | 5.17822869588274 |
| H | 2.29427120622651 | 9.15132244703236 | -0.19374481877006 |
| H | 2.25201895859226 | 8.87476096600960 | -2.68500968503203 |
| H | 0.38433262058565 | 7.59754106396835 | -3.75568761635744 |
| H | -1.44923490008681 | 6.65572806415272 | -2.32429687254515 |
| I | -4.05453105140281 | 6.18109566230373 | 2.66697943854991 |
| I | -4.99370860927401 | 11.13752916362420 | 2.19772728499205 |

Table S53. Cartesian coordinates (in Å) of **1**·2$I_t^-$

| Atom | x | y | z |
|---|---|---|---|
| H | -4.41832202423646 | 8.29272646186457 | -0.47804726189582 |
| H | -6.31895847808617 | 8.44193299799363 | 1.14988945736251 |
| H | 5.39607137194620 | 9.34498067011623 | 0.70225102982188 |
| C | -4.26160832179574 | 8.08770953440805 | 0.58313317048035 |
| H | 5.20184239661417 | 11.58697109506320 | 1.80353883817043 |
| C | -5.31549075034568 | 8.18280124098623 | 1.49947329376106 |
| O | -1.95684908078148 | 7.69281321085829 | 0.10689846860291 |
| C | 4.57656843392358 | 9.55297780946239 | 1.39443401233536 |
| C | -2.96419280181081 | 7.76343831748119 | 0.99918030060269 |
| C | 4.45095280987010 | 10.81211946008610 | 1.98274251377503 |
| H | 3.67003237265196 | 7.58939781241942 | 1.17089748934539 |
| C | 3.60072406982565 | 8.57894684748293 | 1.62588434106883 |
| C | -5.07437535744891 | 7.94893506829500 | 2.85389612818721 |
| C | 3.35277547840059 | 11.08404525478920 | 2.80678122129673 |
| H | 3.21807538836047 | 12.06934350199050 | 3.25797328424778 |
| H | -5.87312592718250 | 8.07788555429320 | 3.58831958988024 |
| Sb | -0.09723836637987 | 7.49099231762955 | 1.02016569301177 |
| C | -2.74107266684916 | 7.42339715843665 | 2.37142873277120 |
| C | 2.55433108881894 | 8.79586845857026 | 2.53041589741124 |
| C | -3.78260917450448 | 7.63056856102218 | 3.28380253424152 |
| C | 2.37089541655055 | 10.11578427487980 | 3.05173194477484 |
| O | -0.38892562849507 | 9.29508675374056 | 1.85069097627204 |
| O | -1.53013471262664 | 6.95513185088610 | 2.75482225887063 |
| O | 1.69592975682020 | 7.81205095718548 | 2.88760006664114 |
| O | 1.31233665185614 | 10.39792791327540 | 3.83629295510199 |
| H | -3.56592201747967 | 7.45023316699719 | 4.33815285564229 |
| I | 1.31491415834309 | 8.93253534307035 | -1.01725284793854 |
| Sb | -0.13093471954601 | 8.89871850744011 | 3.79950199870178 |
| I | -2.32610236641302 | 10.69881789927590 | 4.21670405745551 |