Supporting Information

Dibismuthates as linking units for bis-zwitterions and coordination polymers

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1. Materials and experimental methods

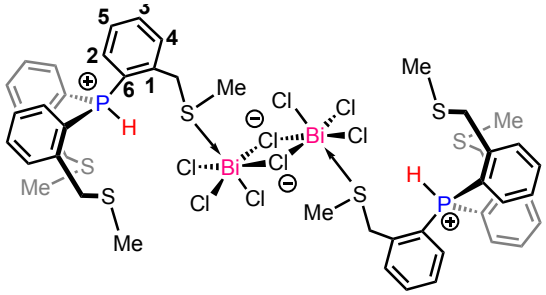
All the reactions reported here were performed using standard Schlenk techniques under a dry nitrogen atmosphere. Sensitive chemicals were stored and weighed in a glove box under nitrogen atmosphere. All the solvents employed were purified and dried by standard methods. Tri(*o*-meththiomethylphenyl) phosphine $P(C_6H_4\text{-}o\text{-}CH_2SCH_3)_3$ (**PS_3**) and **PS_3BiX_3** (X = Cl, Br, I) were prepared according to previously published protocols.[1] All other reagents were purchased from standard chemical suppliers and used without further purification. All the reported new compounds in this paper can be handled on air as solids, however, in solution they slowly decompose (within days time) when not kept under inert atmosphere, presumably due to the hydrolysis of the bismuth centre.

Solution NMR spectra were recorded on a Bruker Avance 400 MHz spectrometer. Chemical shifts are reported in ppm relative to $SiMe_4$ (^1H, ^{13}C), $CFCl_3$ (^{19}F) and 85% H_3PO_4 (^{31}P). Coupling constants are given in Hz. Elemental analyses were performed at Durham University (Chemistry Department) and the Science Centre at London Metropolitan University. X-ray diffraction experiments were carried out at T=120 K (240 K for **1A'**) on a Bruker 3-circle D8 Venture diffractometer with a PHOTON 100 CMOS area detector, using Mo-K_α radiation (λ=0.71073 Å) from an Incoatec IμS microsource with focussing mirrors and a Cryostream (Oxford Cryosystems) open-flow N_2 gas cryostat. The structures were solved by direct methods (SHELXS)[2] and refined by full-matrix least squares using SHELXL software[3] on OLEX2 platform.[4] UV-Vis spectra were recorded on a Cary 5000 UV-Vis-NIR instrument between 250 nm and 800 nm with a data interval of 1.0 nm and scan rate of 600 nm/min. Samples were prepared in dichloromethane with a series of dilutions and analysed at room temperature in quartz cuvettes with a path length of 10 mm. The plotted spectra refer to a concentration of 10^{-6} mol/L.

2. Synthetic procedures

Synthesis of $[(HPS_3)_2(Bi_2Cl_8)]$ (1A)

A solution of hydrogen chloride in dioxane (excess: 1.5 mL of a 4 M solution) was added drop wise at room temperature to a solution of $\mathbf{PS_3}BiCl_3$ (70 mg, 0.09 mmol) in dichloromethane (5 mL). Immediately a colour change (yellow to colourless) was observed. After 30 min stirring at room temperature a colourless solid was isolated and dried *in vacuo*. Crystals of **1A** suitable for an X-ray diffraction analysis were obtained by slow solvent evaporation from a saturated dichloromethane solution. Yield 67 mg (91%).



^{31}P NMR (162 MHz; CD_2Cl_2, 298 K): δ (ppm) = − 20.8 (d, $^1J_{PH}$ = 535.2 Hz);

^{1}H NMR (400 MHz; CD_2Cl_2, 298 K): δ (ppm) = 1.96 (18H, s, CH_3), 4.04 (12H, s, CH_2), 7.28-7.40 (6 H2, m), 7.51-7.59 (6 H5, m), 7.59-7.67 (6 H4, m), 7.74-7.84 (6 H3, m), 10.26 (d, $^1J_{PH}$ = 535.20 Hz, 2 H);

^{13}C NMR (151 MHz; CD_2Cl_2, 298 K): δ (ppm) = 15.6 (s, CH_3), 38.0 (d, $^2J_{PC}$ = 5.7 Hz, CH_2), 115.8 (d, J_{PC} = 85.0 Hz, C6), 129.6 (d, J_{PC} = 13.0 Hz, C5), 133.8 (d, J_{PC} = 10.7 Hz, C4), 135.9 (d, J_{PC} = 1.6 Hz, C3), 136.1 (d, J_{PC} = 10.1 Hz, C2), 142.8 (d, J_{PC} = 7.1 Hz, C1).

Elemental analysis % (calc. %) $C_{48}H_{56}Bi_2P_2S_6Cl_8$: C 33.5 (36.28), H 3.35 (3.55)

The deviation of the carbon content from the calculated value is presumably due to the formation of trace amounts of non-combustible solid carbon residues during the measurement.

Synthesis of $[(HPS_3)_2(Bi_2Br_{5.94}Cl_{2.06})]$ (1B)

A solution of hydrogen chloride in diethyl ether (excess: 0.1 mL of a 2M solution) was added drop wise at room temperature to a suspension of $\mathbf{PS_3}BiBr_3$ (87 mg, 0.098 mmol) in dichloromethane (3 mL). The reaction mixture was stirred for 30 min. at room temperature. Subsequently, a yellow solid was isolated, washed with petrol ether and dried *in vacuo*. Crystals of **1B** suitable for an X-ray diffraction analysis were obtained by solvent evaporation from a dichloromethane solution. Yield 73 mg (80%).

^{31}P NMR (162 MHz; CD_2Cl_2, 298 K): δ (ppm) = − 20.7 (d, $^1J_{PH}$ = 534.7 Hz).

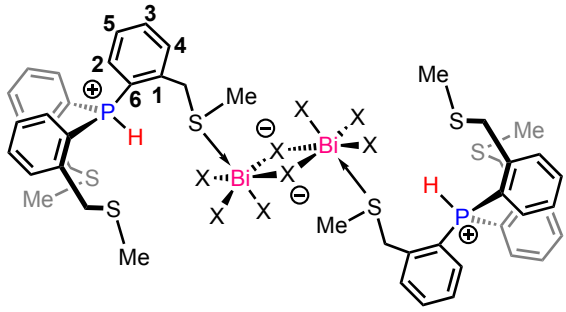
^{1}H NMR (400 MHz; CD_2Cl_2, 298 K): δ (ppm) = 2.03 (18H, s, CH_3), 4.07 (12H, s, CH_2), 7.26-7.41 (6 H_{arom}, m), 7.50-7.61 (6 H_{arom}, m), 7.61-7.71 (6 H_{arom}, m), 7.76-7.88 (6 H_{arom}, m), 10.25 (d, $^{1}J_{PH}$ = 534.7, 2 H);

Due to the low solubility of the compound in common organic solvents reliable ^{13}C NMR data could not be obtained.

Elemental analysis % (calc. %) $C_{48}H_{56}Bi_2P_2S_6Br_{5.94}Cl_{2.06}$: C 31.98 (31.86), 3.14 (3.12).

Synthesis of $[(HPS_3)_2(Bi_2I_{7.19}Cl_{0.81})]$ (1C)

A solution of hydrogen chloride in dioxane (excess: 1.0 mL of a 4 M solution) was added drop wise at room temperature to a solution of **PS_3**BiI_3 (33 mg, 0.032 mmol) in THF (5 mL). Immediately a colour change (dark orange to yellow) was observed. After 30 min stirring at room temperature an orange solid was isolated and dried *in vacuo*. Crystals of **1C** suitable for an X-ray diffraction analysis were obtained by slow solvent evaporation from a saturated THF solution. Yield 15 mg (44%).



^{31}P NMR (162 MHz; CD_2Cl_2, 298 K): δ (ppm) = −21.8 (d, $^{1}J_{PH}$ = 534.7 Hz);

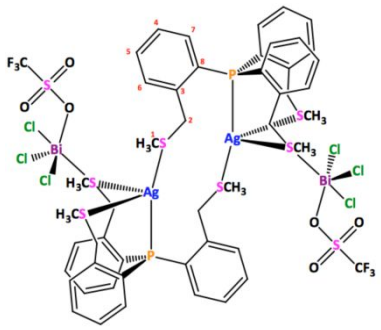
^{1}H NMR (400 MHz; CD_2Cl_2, 298 K): δ (ppm) = 2.03 (18H, s, CH_3), 3.99 (12H, s, CH_2), 7.27-7.46 (6 H_{arom}, m), 7.54-7.72 (12 H_{arom}, m), 7.77-7.95 (6 H_{arom}, m), 10.34 (d, $^{1}J_{PH}$ = 534.70, 2 H);

^{13}C NMR (176 MHz; CD_2Cl_2, 298 K): δ (ppm) = 15.9 (s, CH_3), 37.9 (CH_2), C6 not visible, 129.9 (s, C5), 133.6 (s, C4), 135.6 (s, C3), 136.2 (s, C2), 142.9 (s, C1).

Elemental analysis % (calc. %) $C_{48}H_{56}Bi_2P_2S_6Cl_{0.81}I_{7.19}$: C 25.75 (25.66), H 2.64 (2.51).

Synthesis of $\{[AgPS_3BiCl_3(OTf)]_2(CH_3CN)_2\}_\infty$

PS_3 $BiCl_3$ (100 mg, 0.132 mmol) and silver trifluoromethanesulfonate (34 mg, 0.132 mmol) were combined in a Schlenk flask, acetonitrile (2 mL) was added and the resulting colourless solution was stirred for 1 h at RT under the exclusion of light. Subsequently, the solvent was removed under reduced pressure and the obtained off-white solid was dried *in vacuo*. Yield: 105 mg (78%). Crystals suitable for an X-ray diffraction analysis were obtained from a saturated acetonitrile solution.



^{31}P {^{1}H} NMR (283 MHz; MeCN-d_3, 298 K): δ (ppm) = −33.1 (s);

^{1}H NMR (700 MHz; MeCN-d_3, 298 K): δ (ppm) = 2.15 (6H, s, CH_3), 2.21 (12H, s, CH_3), 3.82 (12H, m, CH_2), 6.80-7.75 (24 $H_{arom.}$, m);

^{13}C NMR (176 MHz; MeCN- d_3, 298 K): δ (ppm) = 17.6 (s, CH_3), 39.9 (d, $^{3}J_{PC}$ = 16.4 Hz, CH_2), 129.9 (d, $^{2}J_{PC}$ = 5.25 Hz, C3), 130.3 (d, $^{3}J_{PC}$ = 4.4 Hz, C4), 132.3 (d, $^{4}J_{PC}$ = 1.3 Hz, C5), 133.9 (d, $^{3}J_{PC}$ = 7.4 Hz, C6), 134.9 (d, $^{2}J_{PC}$ = 1.5 Hz, C7), 140.6 (d, $^{1}J_{PC}$ = 19.7 Hz, C8);

^{19}F {^{1}H} NMR NMR (564 MHz; MeCN-d_3, 298 K): δ (ppm) = −79.3 (s).

Elemental analysis % (calc. %) $C_{54}H_{60}Ag_2Bi_2Cl_6F_6O_6P_2S_8N_2$: C 26.91 (30.71), H 2.56 (2.86), N 0.42 (1.33). We explain the discrepancy between measured and expected results in this analysis by two factors: 1) The loss of acetonitrile during the drying process of the material (according to the single crystal X-ray analysis two acetonitrile molecules per molecular unit are incorporated in the crystal packing in a void, hence solvent can be easily lost into air). 2) The formation of trace amounts of non-combustible solid carbon residues during the measurement also lowers the carbon value.

^{1}H DOSY NMR studies on **2** in CD_2Cl_2 delivered a diffusion coefficient of D = 7.70 10^{-10} m^2 s^{-1} and a hydrodynamic radius of r = 6.87 Å. Analogous experiments employing the **PS_3**$BiCl_3$ starting material resulted D = 1.02 10^{-9} m^2 s^{-1} and a hydrodynamic radius of r = 5.12 Å. These lead to spherical volumes of 1359 $Å^3$ and 562 $Å^3$, respectively. Compared to the cell volume of **2** (1785.35(13) $Å^3$) in the solid-state, the solution of compound **2** presumably contains [Ag**PS_3**$BiCl_3$(OTf)] or its dimeric form (as shown above) rather than a polymer.

Reaction of PS_3 with hydrochloric acid

An excess of hydrochloric acid (0.5 mL, 4M in dioxane) was added at room temperature to a solution of **PS_3** (20 mg, 0.045 mmol) in benzene (1 mL). Immediately the formation of a white precipitate was observed. The solvent was decanted and the precipitate was shortly dried *in vacuo*. The obtained white solid was dissolved in CD_2Cl_2 and investigated by solution ^{1}H and ^{31}P NMR spectroscopy.

^{31}P NMR (162 MHz; CD_2Cl_2, 298 K): δ (ppm) = −32.0 ppm (br s);

^{1}H NMR (400 MHz; CD_2Cl_2, 298 K): δ (ppm) = 1.97 (9H, s, CH_3), 3.92 (6H, s, CH_2), 6.03 (1H, br s, PH), 6.93-7.53 (12 H_{arom}, broad multiplets);

3. Solution NMR spectra

NMR spectra of 1A

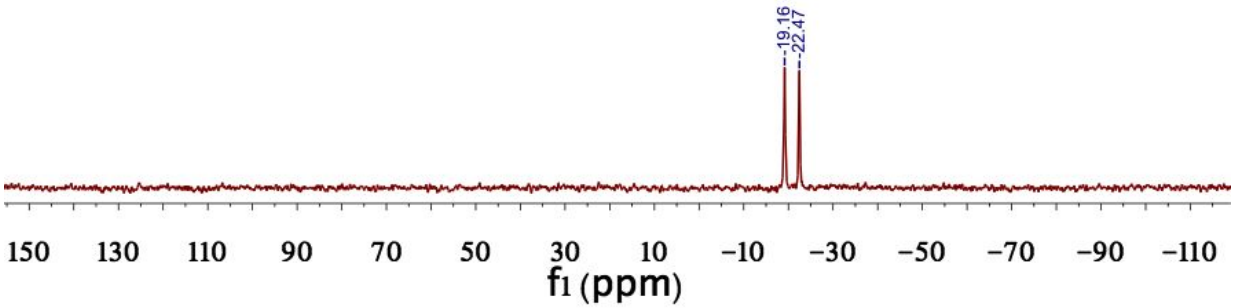


Figure S1: **^{31}P NMR** (CD_2Cl_2, 298 K) of **1A**.

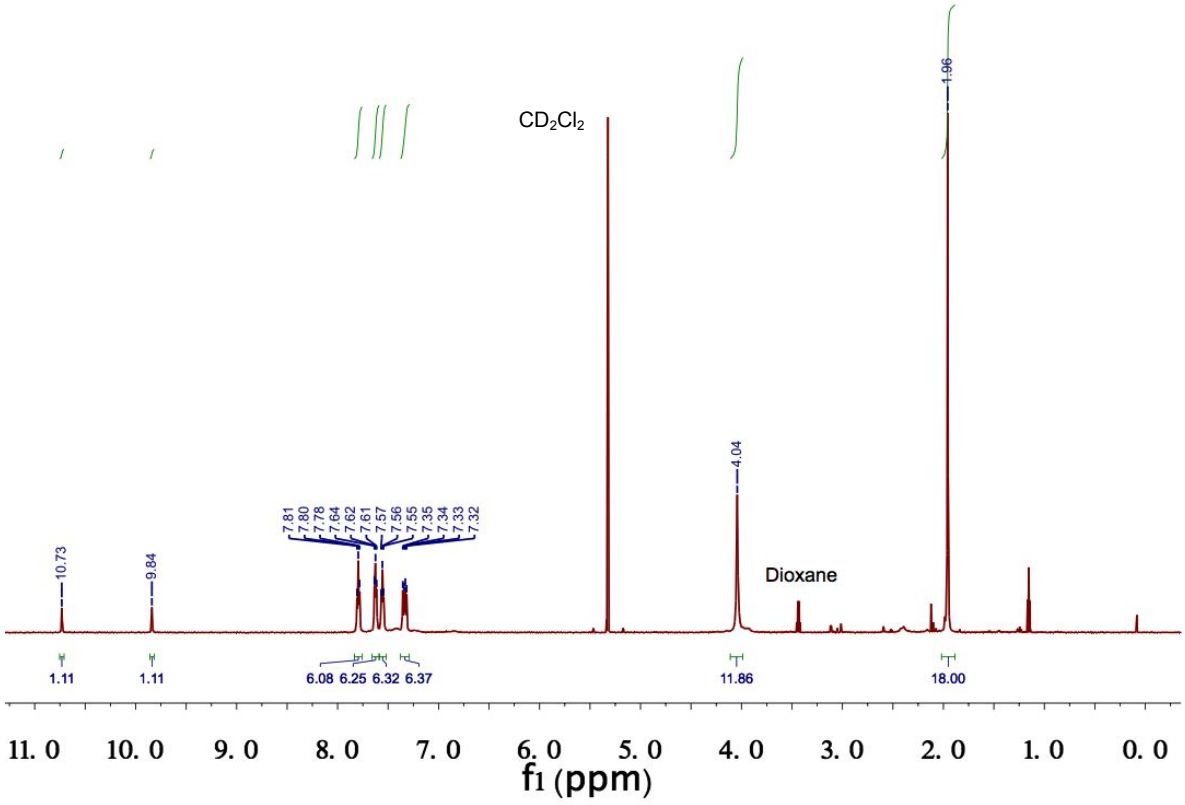


Figure S2: **^{1}H NMR** (CD_2Cl_2, 298 K) of **1A**.

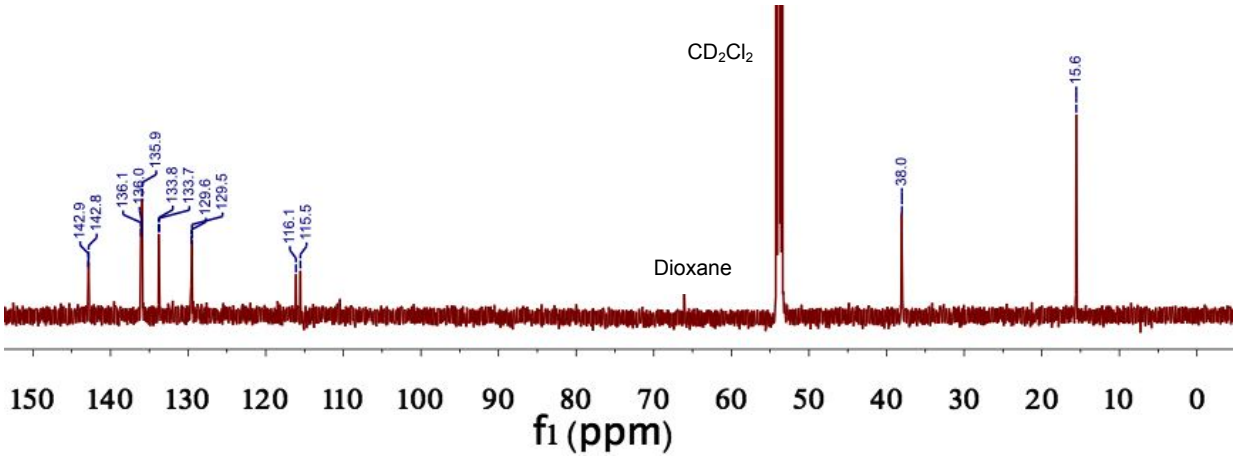


Figure S3: **^{13}C NMR** (CD_2Cl_2, 298 K) of **1A**.

NMR spectra of 1B

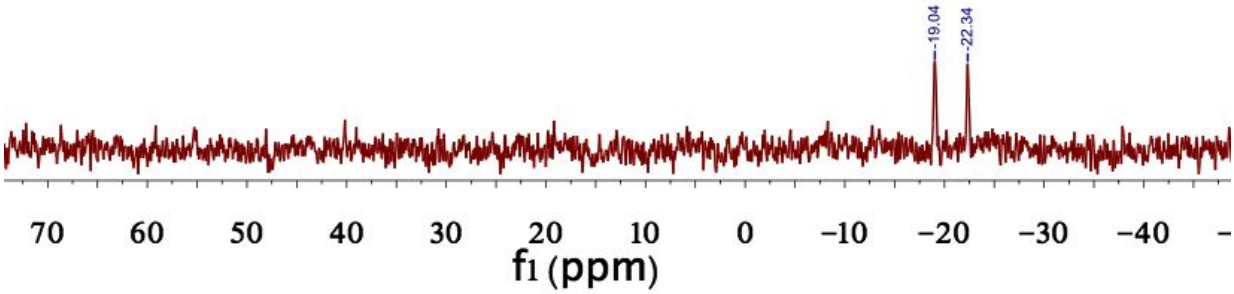


Figure S4: ^{31}**P NMR** (CD_2Cl_2, 298 K) of **1B**.

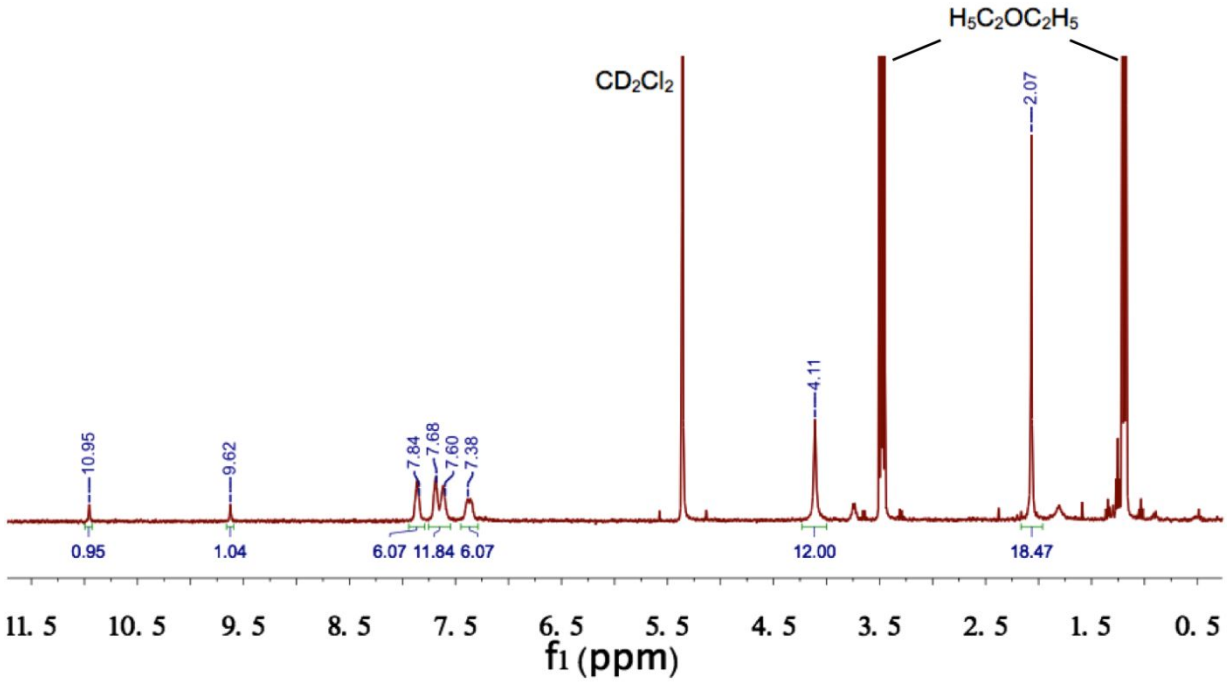


Figure S5: ^{1}**H NMR** (CD_2Cl_2, 298 K) of **1B**.

NMR spectra IC

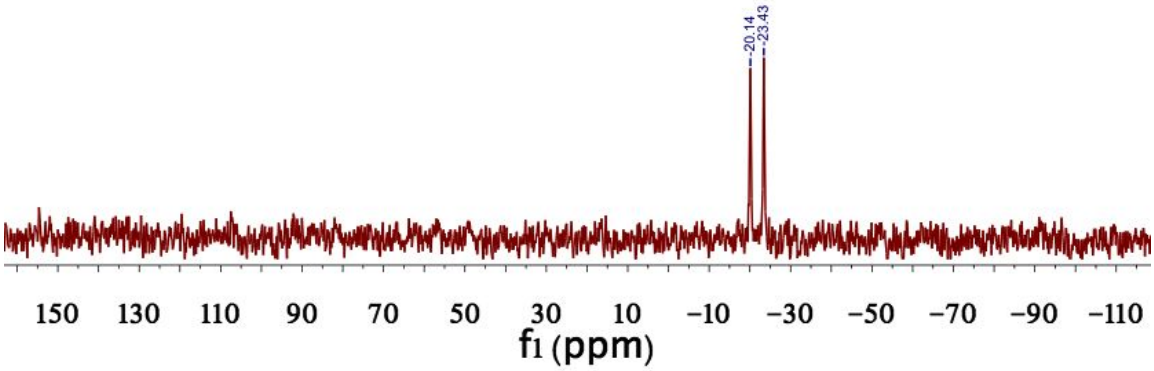


Figure S6: **^{31}P NMR** (CD_2Cl_2, 298 K) of **1C**.

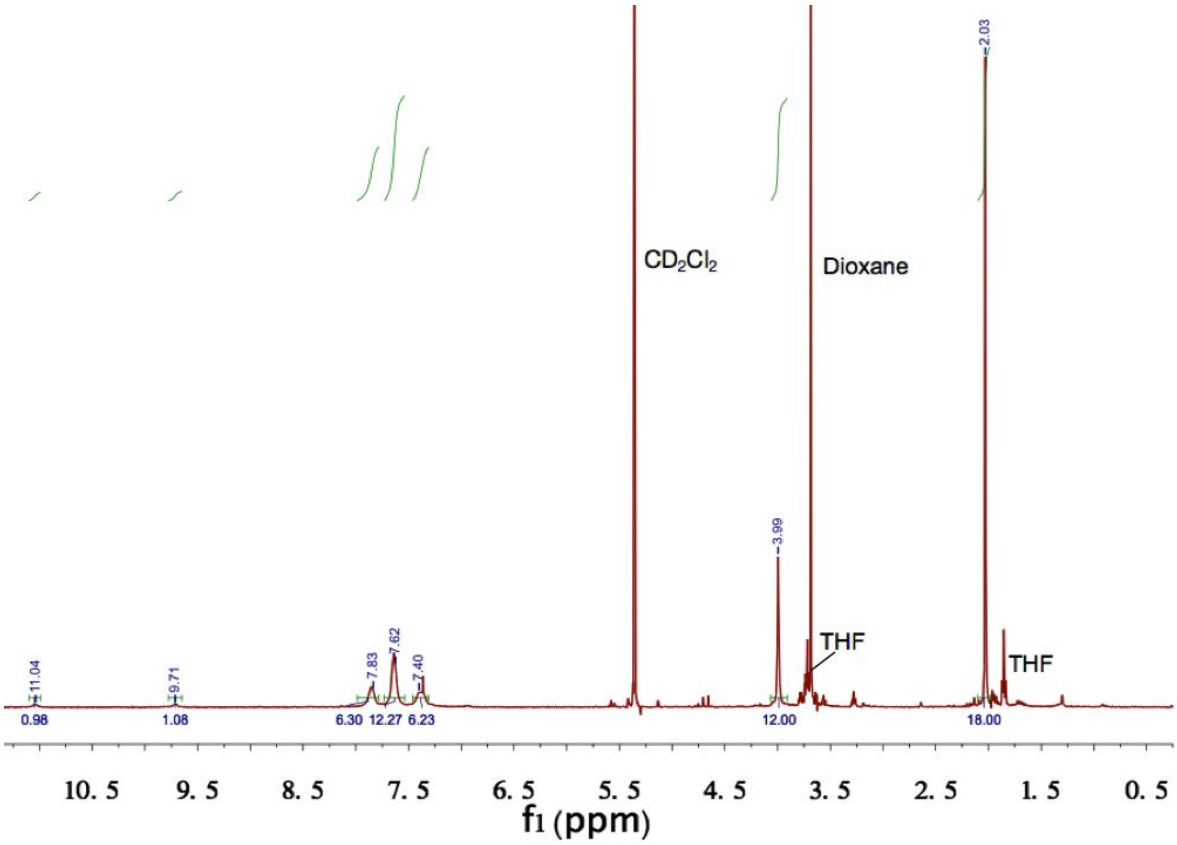


Figure S7: **^{1}H NMR** (CD_2Cl_2, 298 K) of **1C**.

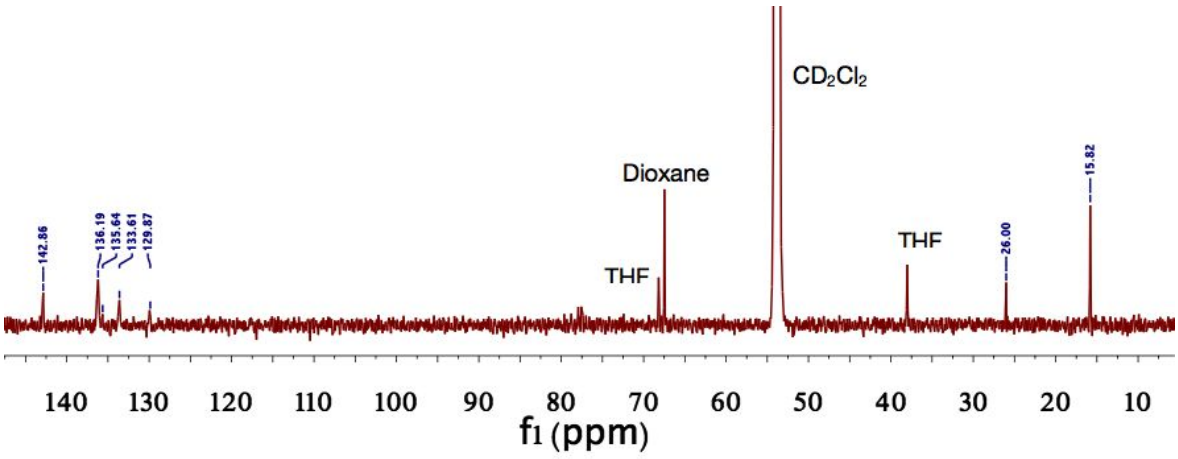


Figure S8: **^{13}C NMR** (CD_2Cl_2, 298 K) of **1C**.

NMR spectra of 2

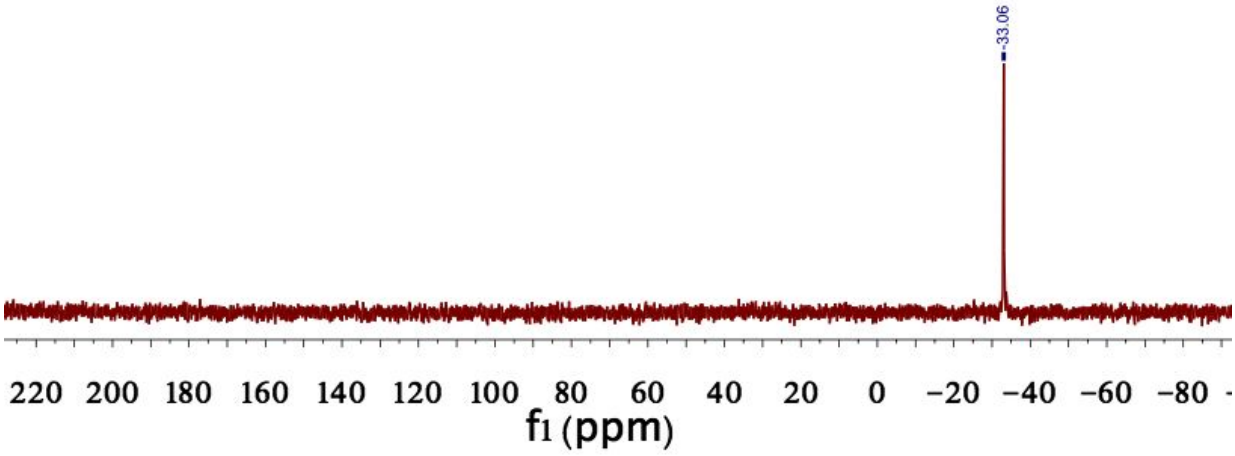


Figure S9: **^{31}P {^{1}H} NMR** (MeCN-d_3, 298 K) of **2**.

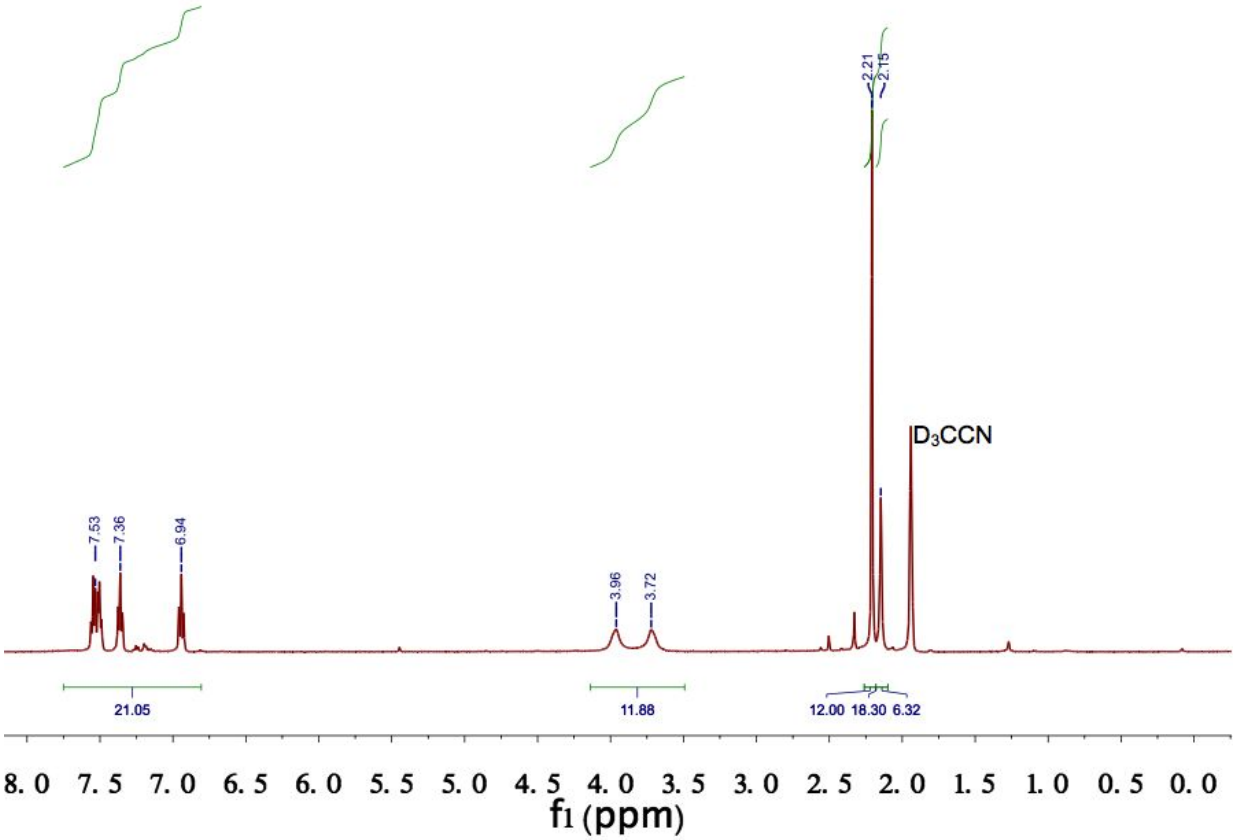


Figure S10: **^{1}H NMR** (MeCN- d_3, 298 K) of **2**.

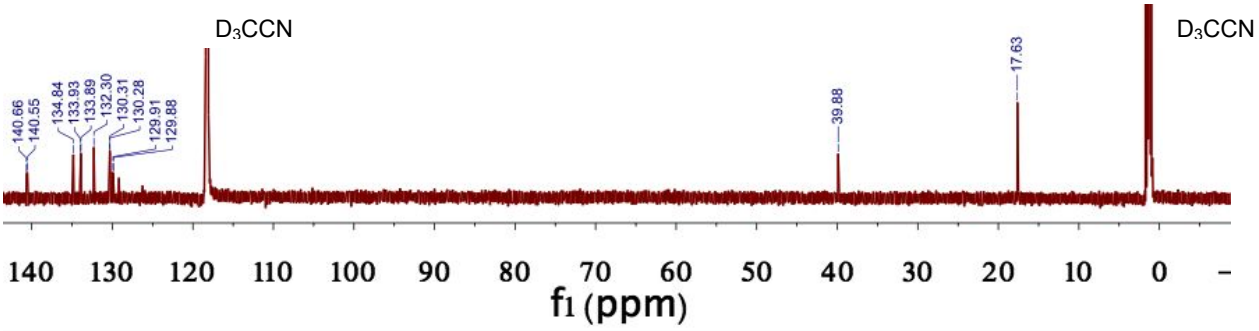


Figure S11: **^{13}C NMR** (MeCN- d_3, 298 K) of **2**.

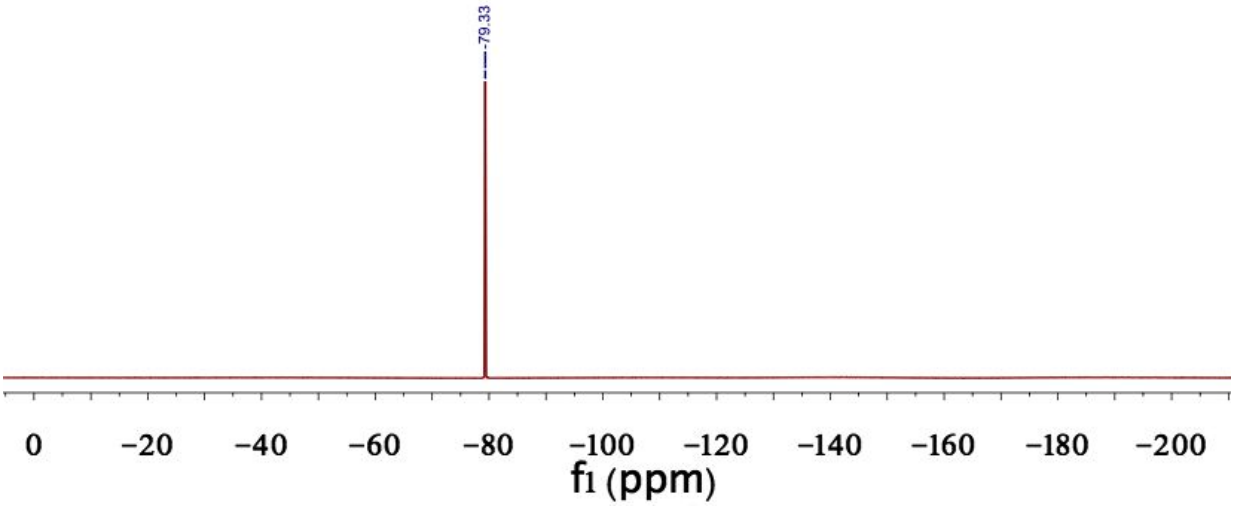


Figure S12: **^{19}F NMR** (MeCN- d_3, 298 K) of **2**.

4. X-ray structure analyses

Table S1. Crystal data and experimental details

Compound	**1A'**	**1A''**	**1A'''**	**1B**	**1C**	**2**
CCDC	1998215	1998469	1998214	1998216	1998217	1998218
Formula	$C_{48}H_{56}Bi_2Cl_8P_2S_6$	$C_{48}H_{56}Bi_2Cl_8P_2S_6$	$C_{48}H_{56}Bi_2Cl_8P_2S_6$	$C_{48}H_{56}Bi_2Br_{8-x}Cl_xP_2S_6$ (x = 2.06)	$C_{48}H_{56}Bi_2Cl_yI_{8-y}P_2S_6$ (y = 0.81)	$C_{54}H_{60}Ag_2Bi_2Cl_6F_6N_2O_6P_2S_8$
$D_{calc.}$/ g cm^{-3}	1.759	1.777	1.798	2.029	2.328	1.964
m/mm^{-1}	6.51	6.58	6.65	10.09	9.26	6.02
Formula Weight	1588.78	1588.78	1588.78	1852.88	2246.31	2111.86
Size/mm^3	0.31×0.30×0.25	0.47×0.30×0.27	0.49×0.33×0.31	0.13×0.09×0.05	0.22×0.03×0.02	0.35×0.14×0.12
T/K	240	120	120	120	120	120
Crystal System	monoclinic	monoclinic	triclinic	triclinic	monoclinic	triclinic
Space Group	$P2_1/n$	$P2_1/n$	$P\bar{1}$	$P\bar{1}$	$P2_1/n$	$P\bar{1}$
a/Å	10.8174(3)	10.3673(7)	10.6941(10)	10.8071(6)	11.2567(4)	12.3102(5)
b/Å	20.8896(6)	19.4377(13)	13.2591(12)	13.3473(7)	22.3546(9)	12.7638(5)
c/Å	13.2828(4)	14.8867(10)	20.711(2)	21.0332(11)	12.7369(5)	13.9089(6)
a/°	90	90	89.945(4)	90.140(2)	90	65.3085(14)
b/°	92.033(1)	98.263(3)	89.775(4)	90.299(2)	90.1767(13)	66.0324(14)
g/°	90	90	87.805(4)	90.999(2)	90	88.7570(15)
V/Å^3	2999.64(15)	2968.8(3)	2934.5(5)	3033.4(3)	3205.1(2)	1785.35(13)
Z	2	2	2	2	2	1
Q_{max}/°	29.6	33.7	30.0	27.9	32.5	33.0
Reflections total	48241	78876	57661	58840	80633	46661
Reflections unique	8403	11843	17149	14468	11582	13419
Refls with $I > 2\sigma(I)$	6737	9895	13879	11220	9218	11888
R_{int}	0.0409	0.0552	0.0785	0.0608	0.0448	0.0308
Parameters	306	319	597	624	332	405
Restraints	0	5	466	600	2	0
$\Delta\rho_{max,min}$/e Å^{-3}	0.72, -0.76	1.46, -1.01	5.80, -7.67	1.71, -0.95	1.14, -1.07	0.82, -0.76
Goodness of fit	1.042	1.036	1.139	1.032	1.025	1.034
wR_2 (all data)	0.0544	0.0539	0.2143	0.0762	0.0509	0.0479
wR_2 [$I > 2\sigma(I)$]	0.0516	0.0514	0.1980	0.0697	0.0472	0.0458
R_1 (all data)	0.0410	0.0359	0.0887	0.0694	0.0436	0.0336
R_1 [$I > 2\sigma(I)$]	0.0267	0.0240	0.0741	0.0434	0.0256	0.0251

At room temperature, complex **1A** crystallizes in two different polymorphic forms (**1A'** and **1A''**). Both have monoclinic space group $P2_1/n$, with one-half of the centrosymmetric molecule per asymmetric unit. Form **1A'** is enantiotropic: between 220 and 200 K it undergoes a phase transition to a triclinic (space group $P\bar{1}$) form **1A'''**, which then persists down to 120 K, at which temperature the crystal structure of **1A'''** was determined. During the transition, a single crystal of **1A'** converts into a two-component pseudo-merohedral twin; the twinning is by a 180° rotation around the former unique monoclinic axis [note that the *reduced* cell of **1A'''** differs from that of **1A'** by circular permutation of axes, so that the monoclinic axis *y* of **1A'** becomes *z* in **1A'''**]. In **1A'''**, the asymmetric unit comprises two halves of crystallographically non-equivalent centrosymmetric molecules (Figure S13). The transition is fully reversible: on warming the twin reverted to a *single* crystal of **1A'**, full structure determination of which was then carried out at 240 K. On the contrary, form **1A''** showed no phase transition on cooling from room temperature to 120 K (Table S2).

The triclinic crystal structure of **1B** closely resembles **1A'''**; with the asymmetric unit also comprising two halves of centrosymmetric molecules. **1B** can be described as pseudo-monoclinic (and thus similar to **1A'**): the structure can be solved and refined in space group $P2_1/n$ (with unique axis *z*), albeit with irreducibly higher R-factor (0.09 cf. 0.043). Also like **1A'''**, **1B** shows pseudo-merohedral twinning by a 180° rotation around the pseudo-monoclinic axis (*z*). The positions of Cl and Br atoms could not be resolved, therefore they were refined as single atoms with mixed scattering factors; the relative occupancies were refined independently for each site.

The monoclinic structure of **1C** resembled that of **1A'**. In this case, Cl and I atoms at each site were resolved and refined separately, again with relative occupancies refined independently for each site, with Cl…I separations of 0.36 – 0.45 Å.

Table S2. Unit cell parameters of 1A polymorphs at variable temperature

Form	T, K	*a,* Å	*b,* Å	*c,* Å	α, °	β, °	γ, °	*V*, Å^3
1A'	240	10.821(3)	20.876(4)	13.292(3)	90	92.13(1)	90	3000.8(1.5)
1A'	220	10.816(3)	20.853(6)	13.287(4)	90	92.16(2)	90	2995(2)
1A'''	200	10.789(3)	13.285(4)	20.797(6)	90.03(2)	90.30(2)	92.35(2)	2978(1)
1A'''	120	10.694(1)	13.259(1)	20.711(2)	89.945(4)	89.775(4)	87.805(4)	2934.5(7)
1A'	240[a]	10.8174(3)	20.8896(6)	13.2828(4)	90	92.033(1)	90	2999.6(2)
1A''	290	10.422(5)	19.722(9)	14.942(7)	90	98.30(3)	90	3039(3)
1A''	240	10.414(3)	19.629(5)	14.924(4)	90	98.57(2)	90	3016.5(1.8)
1A''	200	10.394(3)	19.572(5)	14.915(4)	90	98.59(2)	90	3000.1(1.6)
1A''	180	10.385(4	19.529(7)	14.901(5)	90	98.54(2)	90	2989(2)
1A''	150	10.365(3)	19.484(6)	14.888(4)	90	98.39(2)	90	2975(2)
1A''	120	10.367(1)	19.438(1)	14.887(1)	90	98.263(3)	90	2968.8(3)

[a] After rewarming

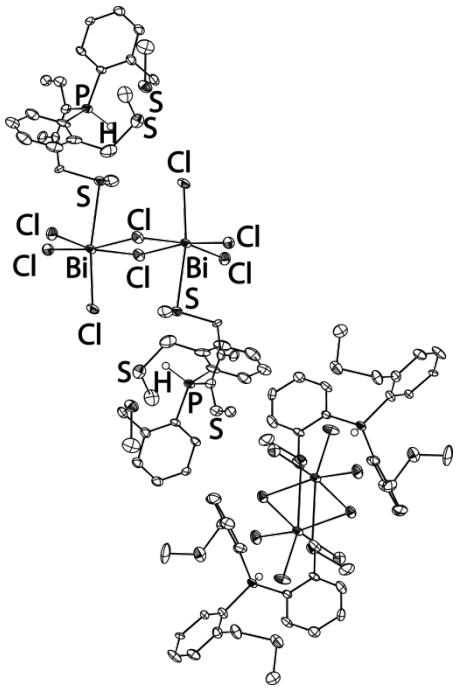


Figure S13: ORTEP representation of **1A'''**. Thermal ellipsoids are drawn at 50% probability. Carbon-bonded hydrogen atoms have been omitted for clarity.

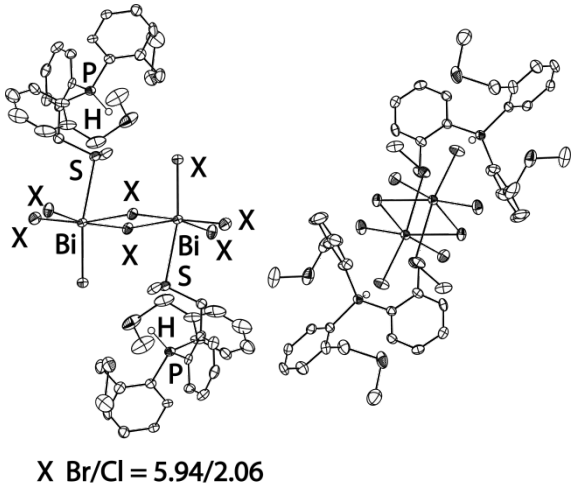


Figure S14: ORTEP representation of **1B**. Thermal ellipsoids are drawn at 50% probability. Carbon-bonded hydrogen atoms have been omitted for clarity.

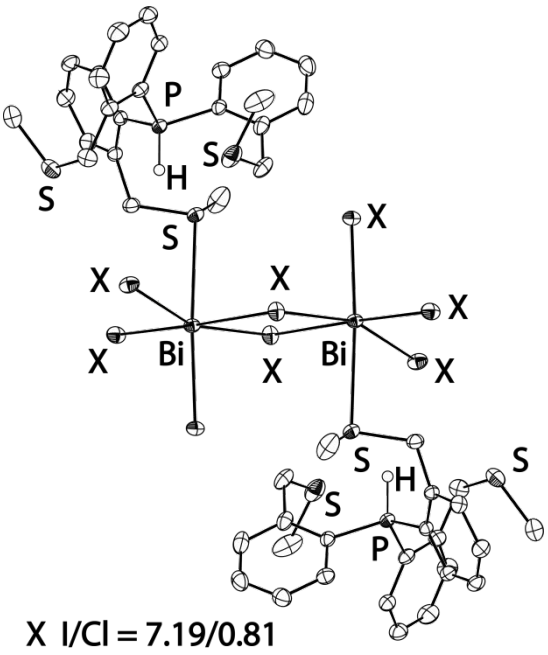
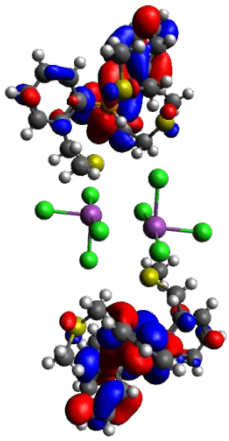
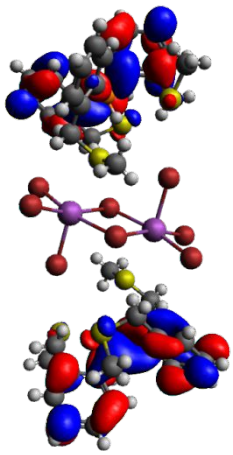
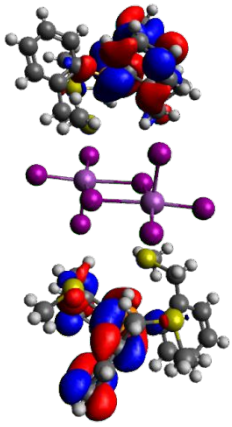
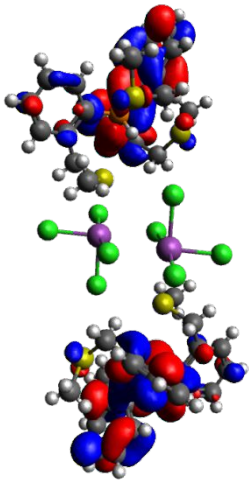
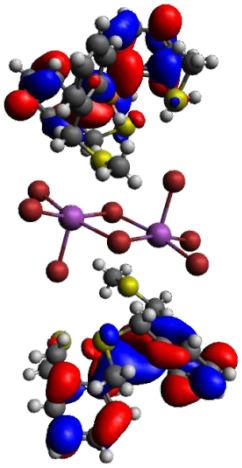
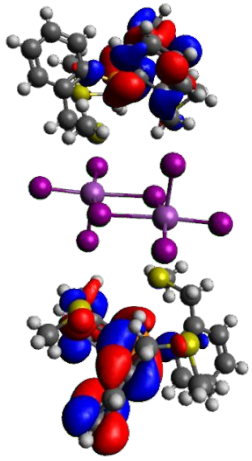


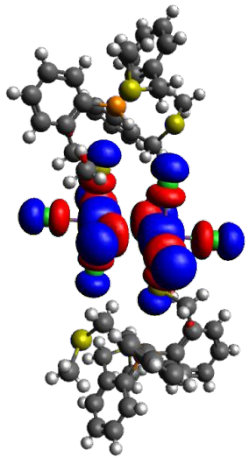
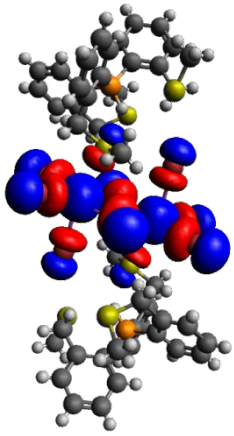
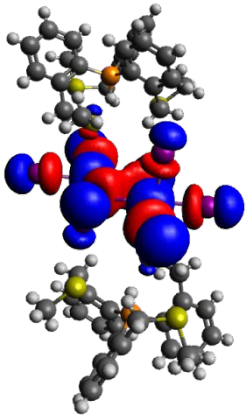
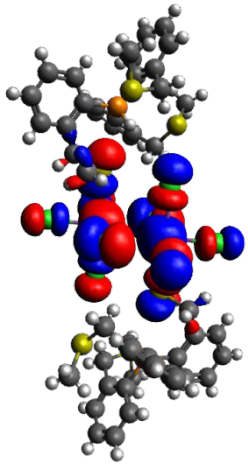
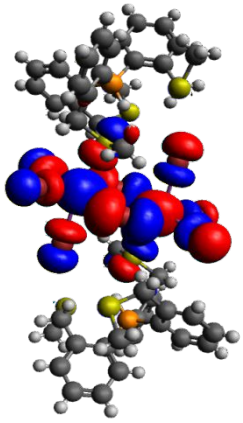
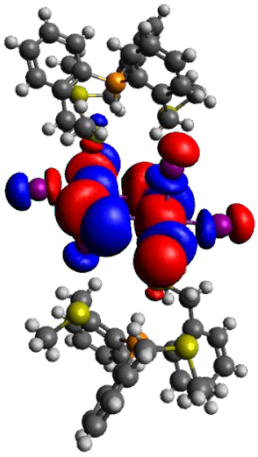
Figure S15: ORTEP representation of **1C**. Thermal ellipsoids are drawn at 50% probability. Carbon-bonded hydrogen atoms have been omitted for clarity.

5. Computational details

The computations were performed with the Gaussian 09 suite of programs.[5] All structures were optimised using the ωB97XD functionals. We employed the def2-SVP basis set implemented in Gaussian 09 or thee all valence cc-pVDZ basis set for H, C, P, S, Cl, O, and Br, while for Bi and I the cc-pVDZ-PP basis sets including pseudopotentials for the modelling of relativistic effects were used. For the anionic species the aug-cc-pVDZ-(PP) basis sets were used. Similar levels of theory have been successfully employed for similar systems.[1, 6] The basis sets with pseudo potentials were obtained from the EMSL Basis Set Library (https://www.basissetexchange.org/).[7-8] The effect of solvents has been simulated using the polarizable continuum model with dichloromethane as solvent. At each of the optimised structures vibrational analysis was performed to check whether the stationary point located is a minimum or a saddle point of the potential energy hypersurface. The time dependent DFT calculations were employed to simulate the UV-VIS spectra with the first 20 excitations at the TD-ωB97XD/def2-SVP level including PCM solvent model with DCM as a solvent, utilizing the solid-state structures. For Wiberg Bond Indices and NPA charges the NBO program version 3.1 was used.[9] The AIM analysis was obtained with the Multiwfn code.[10] The plotting of the orbitals was performed with the AVOGADRO program (www.avogadro.cc).

Table S3: Selected orbitals of the bis-zwitterions at the ωB97XD/def2-SVP level with the contour value of 0.02.

	[HPS$_3$BiCl$_4$]$_2$	[HPS$_3$BiBr$_4$]$_2$	[HPS$_3$BiI$_4$]$_2$
LUMO+1			
LUMO+1 Energy (eV)	-0,003	-0,075	0,055
LUMO			
LUMO Energy (eV)	-0,004	-0,081	0,044

HOMO			
HOMO Energy (eV)	-7,844	-7,752	-6,577
HOMO-1			
HOMO-1 Energy (eV)	-7,943	-7,905	-6,675

[HPS_3BiCl_4]$_2$ B3LYP/def2-SVP (PCM)

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.7571 eV 330.00 nm f=0.0001 <S**2>=0.000
325 -> 328 -0.32207
326 -> 327 0.60191
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -9041.93271949
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.7573 eV 329.98 nm f=0.0003 <S**2>=0.000
325 -> 327 -0.32206
326 -> 328 0.59966

Excited State 3: Singlet-A 3.8054 eV 325.81 nm f=0.0033 <S**2>=0.000
325 -> 329 0.35909
325 -> 330 -0.12739
326 -> 327 0.10804
326 -> 329 -0.21271
326 -> 330 0.53034

Excited State 4: Singlet-A 3.8054 eV 325.81 nm f=0.0224 <S**2>=0.000
325 -> 329 0.13222
325 -> 330 0.34692
326 -> 328 -0.10044
326 -> 329 0.54049
326 -> 330 0.20898

Excited State 5: Singlet-A 3.8429 eV 322.63 nm f=0.0010 <S**2>=0.000
323 -> 327 -0.43232
323 -> 328 -0.16883
324 -> 327 0.18431
324 -> 328 0.43796

Excited State 6: Singlet-A 3.8429 eV 322.63 nm f=0.0062 <S**2>=0.000
323 -> 327 -0.18157
323 -> 328 0.43947
324 -> 327 -0.43162
324 -> 328 0.17121

Excited State 7: Singlet-A 3.8761 eV 319.87 nm f=0.0015 <S**2>=0.000
325 -> 327 0.59961
326 -> 328 0.34386

Excited State 8: Singlet-A 3.8768 eV 319.81 nm f=0.0000 <S**2>=0.000
322 -> 327 0.10256
325 -> 328 0.59954
326 -> 327 0.33817

Excited State 9: Singlet-A 3.9401 eV 314.68 nm f=0.0000 <S**2>=0.000
321 -> 328 0.40294

321 -> 329 -0.14448
322 -> 327 0.40541
322 -> 330 0.14761
325 -> 328 -0.13366
325 -> 329 -0.22185
326 -> 330 0.19917

Excited State 10: Singlet-A 3.9407 eV 314.62 nm f=0.0190 <S**2>=0.000
321 -> 327 0.41646
321 -> 330 0.14257
322 -> 328 0.41091
322 -> 329 -0.15749
325 -> 327 -0.13483
325 -> 330 0.20071
326 -> 329 -0.17027

Excited State 11: Singlet-A 3.9551 eV 313.48 nm f=0.0000 <S**2>=0.000
321 -> 328 0.19441
322 -> 327 0.19466
325 -> 329 0.53621
326 -> 330 -0.34669

Excited State 12: Singlet-A 3.9557 eV 313.43 nm f=0.0085 <S**2>=0.000
321 -> 327 -0.17498
322 -> 328 -0.17311
325 -> 330 0.55359
326 -> 329 -0.34595

Excited State 13: Singlet-A 3.9895 eV 310.78 nm f=0.0008 <S**2>=0.000
323 -> 330 0.45998
324 -> 329 0.46838

Excited State 14: Singlet-A 3.9897 eV 310.76 nm f=0.0218 <S**2>=0.000
323 -> 329 0.46656
323 -> 330 0.10264
324 -> 330 0.46124

Excited State 15: Singlet-A 4.1795 eV 296.65 nm f=0.0002 <S**2>=0.000
321 -> 328 -0.17437
321 -> 329 -0.45885
322 -> 327 -0.16459
322 -> 330 0.46196

Excited State 16: Singlet-A 4.1799 eV 296.62 nm f=0.0387 <S**2>=0.000
321 -> 327 0.16320
321 -> 330 -0.45823
322 -> 328 0.17703
322 -> 329 0.46202

Excited State 17: Singlet-A 4.2794 eV 289.73 nm f=0.0018 <S**2>=0.000
325 -> 332 0.29593
326 -> 331 0.62428

Excited State 18: Singlet-A 4.2804 eV 289.65 nm f=0.0000 <S**2>=0.000
325 -> 331 0.30586
326 -> 332 0.61915

Excited State 19: Singlet-A 4.3357 eV 285.96 nm f=0.0000 <S**2>=0.000
323 -> 327 0.39387
323 -> 328 -0.29494
324 -> 327 -0.30412
324 -> 328 0.40438

Excited State 20: Singlet-A 4.3358 eV 285.96 nm f=0.0000 <S**2>=0.000
323 -> 327 0.30710
323 -> 328 0.40333
324 -> 327 0.39483
324 -> 328 0.29200

[HPS_3BiBr_4]$_2$ B3LYP/def2-SVP (PCM)

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.6462 eV 340.03 nm f=0.0001 <S**2>=0.000
397 -> 400 -0.12922
398 -> 399 0.67914
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -25952.3765732
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.6515 eV 339.55 nm f=0.0011 <S**2>=0.000
397 -> 399 -0.14150
398 -> 400 0.67701

Excited State 3: Singlet-A 3.7516 eV 330.48 nm f=0.0049 <S**2>=0.000
394 -> 399 -0.18981
395 -> 400 -0.20439
397 -> 399 0.55681
398 -> 400 0.11636
398 -> 402 -0.23837

Excited State 4: Singlet-A 3.7555 eV 330.14 nm f=0.0000 <S**2>=0.000
394 -> 400 -0.20615
395 -> 399 -0.21735
397 -> 400 0.52352
398 -> 399 0.10803
398 -> 401 0.28245

Excited State 5: Singlet-A 3.7700 eV 328.87 nm f=0.0000 <S**2>=0.000
397 -> 400 -0.29469
397 -> 402 0.20563
398 -> 401 0.58618

Excited State 6: Singlet-A 3.7746 eV 328.47 nm f=0.0137 <S**2>=0.000

397 -> 399 0.24243
397 -> 401 0.22242
398 -> 402 0.60613

Excited State 7: Singlet-A 3.8062 eV 325.75 nm f=0.0006 <S**2>=0.000
393 -> 399 0.44821
394 -> 400 0.11543
395 -> 399 0.14555
396 -> 400 0.44671

Excited State 8: Singlet-A 3.8064 eV 325.73 nm f=0.0148 <S**2>=0.000
393 -> 400 0.44239
394 -> 399 0.11289
395 -> 400 0.14210
396 -> 399 0.45503

Excited State 9: Singlet-A 3.8355 eV 323.26 nm f=0.0068 <S**2>=0.000
393 -> 400 -0.11050
394 -> 399 0.39778
394 -> 401 0.10250
395 -> 400 0.38842
397 -> 399 0.30587
397 -> 401 -0.14442
398 -> 400 0.12917

Excited State 10: Singlet-A 3.8381 eV 323.03 nm f=0.0000 <S**2>=0.000
393 -> 399 -0.11131
394 -> 400 0.39588
395 -> 399 0.38294
395 -> 401 0.10290
397 -> 400 0.32484
397 -> 402 0.13452
398 -> 399 0.12750

Excited State 11: Singlet-A 3.9003 eV 317.88 nm f=0.0066 <S**2>=0.000
394 -> 399 0.10815
395 -> 400 0.10295
397 -> 401 0.62234
398 -> 402 -0.24097

Excited State 12: Singlet-A 3.9019 eV 317.75 nm f=0.0001 <S**2>=0.000
397 -> 402 0.62824
398 -> 401 -0.23791

Excited State 13: Singlet-A 4.0418 eV 306.75 nm f=0.0004 <S**2>=0.000
394 -> 402 -0.46434
395 -> 399 -0.10678
395 -> 401 0.47855

Excited State 14: Singlet-A 4.0432 eV 306.65 nm f=0.0422 <S**2>=0.000
394 -> 399 0.10465
394 -> 401 -0.47137

395 -> 402 0.47263
397 -> 401 -0.10008

Excited State 15: Singlet-A 4.0924 eV 302.96 nm f=0.0350 <S**2>=0.000
393 -> 400 0.10422
393 -> 402 -0.44278
393 -> 403 0.10193
396 -> 401 0.48573

Excited State 16: Singlet-A 4.0933 eV 302.90 nm f=0.0010 <S**2>=0.000
393 -> 401 -0.45437
393 -> 404 -0.10053
396 -> 400 -0.11900
396 -> 402 0.47520

Excited State 17: Singlet-A 4.1911 eV 295.83 nm f=0.0090 <S**2>=0.000
397 -> 404 -0.12668
398 -> 403 0.66257

Excited State 18: Singlet-A 4.1946 eV 295.58 nm f=0.0000 <S**2>=0.000
397 -> 403 -0.14381
398 -> 404 0.65239
398 -> 405 -0.10325

Excited State 19: Singlet-A 4.2190 eV 293.87 nm f=0.0000 <S**2>=0.000
389 -> 399 -0.16739
391 -> 400 0.30807
392 -> 399 0.53659
396 -> 400 -0.12839

Excited State 20: Singlet-A 4.2212 eV 293.72 nm f=0.0069 <S**2>=0.000
389 -> 400 -0.20261
391 -> 399 0.35963
392 -> 400 0.47156
393 -> 400 0.13987
396 -> 399 -0.18790

[HPS_3BiI_4]$_2$ B3LYP/def2-SVP (PCM)

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.8273 eV 438.52 nm f=0.0001 <S**2>=0.000
357 -> 360 -0.13638
358 -> 359 0.68292
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -7743.58440740
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.8371 eV 437.01 nm f=0.0062 <S**2>=0.000
357 -> 359 -0.17113
358 -> 360 0.67341
358 -> 361 0.10550

Excited State 3: Singlet-A 2.9036 eV 427.00 nm f=0.0029 <S**2>=0.000
357 -> 359 0.67046
358 -> 360 0.15534

Excited State 4: Singlet-A 2.9125 eV 425.69 nm f=0.0000 <S**2>=0.000
357 -> 360 0.67623
357 -> 361 0.12226
358 -> 359 0.12685

Excited State 5: Singlet-A 2.9362 eV 422.26 nm f=0.0015 <S**2>=0.000
357 -> 361 -0.25731
357 -> 362 0.13561
358 -> 361 0.57343
358 -> 362 -0.26731

Excited State 6: Singlet-A 2.9375 eV 422.07 nm f=0.0014 <S**2>=0.000
357 -> 361 0.12915
357 -> 362 0.26162
358 -> 361 0.26007
358 -> 362 0.57644

Excited State 7: Singlet-A 3.0445 eV 407.24 nm f=0.0001 <S**2>=0.000
357 -> 359 -0.10185
357 -> 361 0.54764
357 -> 362 -0.31516
358 -> 361 0.26064
358 -> 362 -0.10342

Excited State 8: Singlet-A 3.0456 eV 407.10 nm f=0.0001 <S**2>=0.000
357 -> 360 -0.11121
357 -> 361 0.31312
357 -> 362 0.54763
358 -> 361 -0.10576
358 -> 362 -0.26174

Excited State 9: Singlet-A 3.2900 eV 376.86 nm f=0.0001 <S**2>=0.000
357 -> 364 0.22397
358 -> 363 0.66462

Excited State 10: Singlet-A 3.2987 eV 375.86 nm f=0.0139 <S**2>=0.000
357 -> 363 0.27084
358 -> 364 0.64716

Excited State 11: Singlet-A 3.3837 eV 366.41 nm f=0.0012 <S**2>=0.000
357 -> 363 0.64697
358 -> 364 -0.27107

Excited State 12: Singlet-A 3.3918 eV 365.54 nm f=0.0000 <S**2>=0.000
357 -> 364 0.66478
358 -> 363 -0.22448

Excited State 13: Singlet-A 3.4791 eV 356.37 nm f=0.0026 <S**2>=0.000
357 -> 366 -0.15780
358 -> 365 0.67816

Excited State 14: Singlet-A 3.4803 eV 356.24 nm f=0.0001 <S**2>=0.000
357 -> 365 -0.16033
358 -> 366 0.67820

Excited State 15: Singlet-A 3.5573 eV 348.54 nm f=0.0000 <S**2>=0.000
357 -> 365 0.66035
357 -> 366 -0.11715
358 -> 366 0.15659

Excited State 16: Singlet-A 3.5586 eV 348.41 nm f=0.0046 <S**2>=0.000
357 -> 365 0.11835
357 -> 366 0.66467
357 -> 369 -0.10360
358 -> 365 0.15560

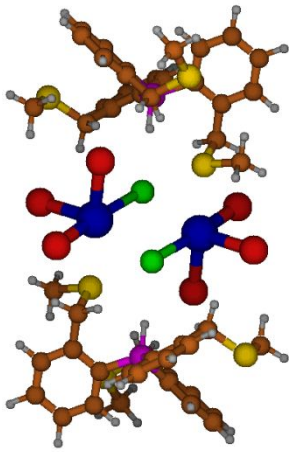
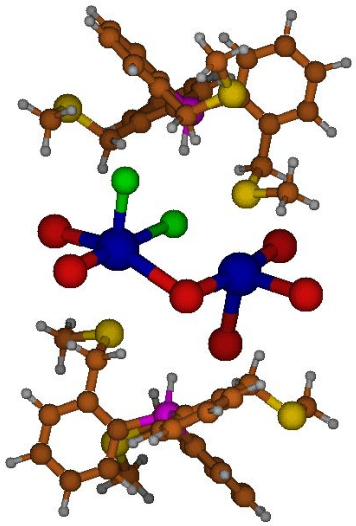
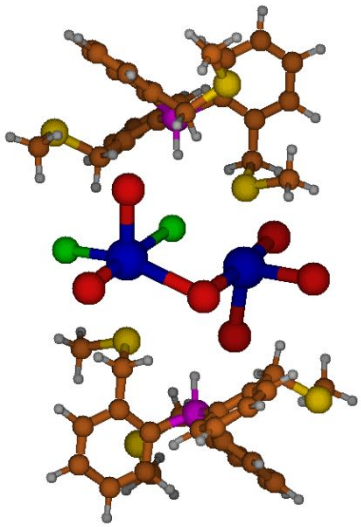
Excited State 17: Singlet-A 3.6808 eV 336.84 nm f=0.0000 <S**2>=0.000
357 -> 370 -0.10920
358 -> 367 0.44538
358 -> 368 -0.24473
358 -> 369 -0.43836
358 -> 371 -0.13367

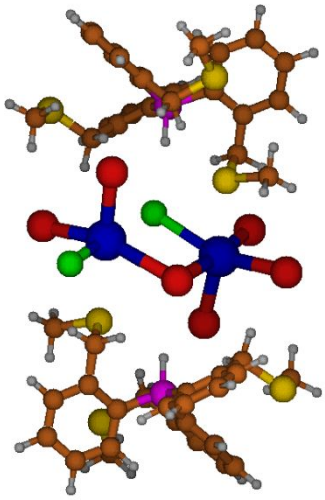
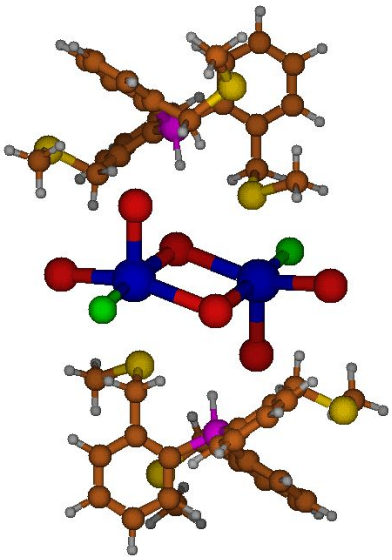
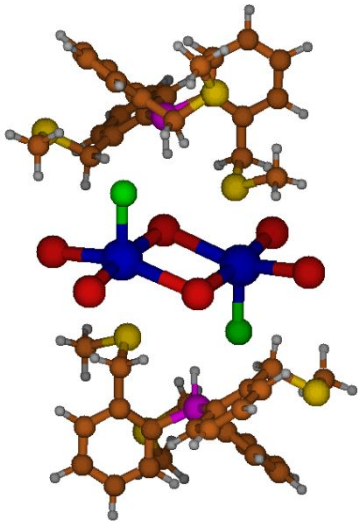
Excited State 18: Singlet-A 3.7225 eV 333.07 nm f=0.0098 <S**2>=0.000
357 -> 367 -0.33417
357 -> 368 0.17276
357 -> 369 0.23209
358 -> 367 0.15553
358 -> 368 0.33425
358 -> 370 0.39566

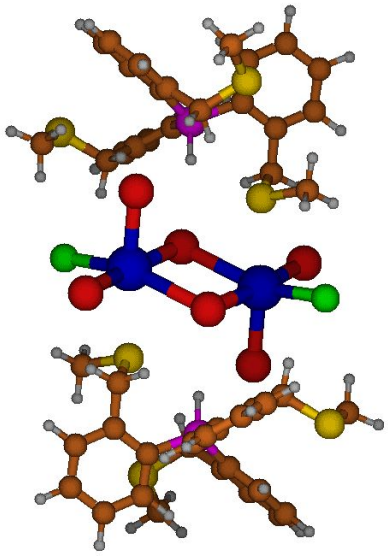
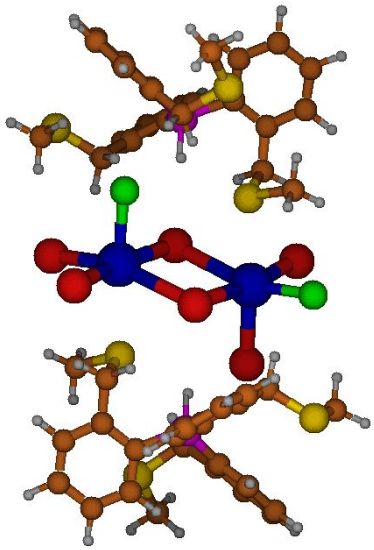
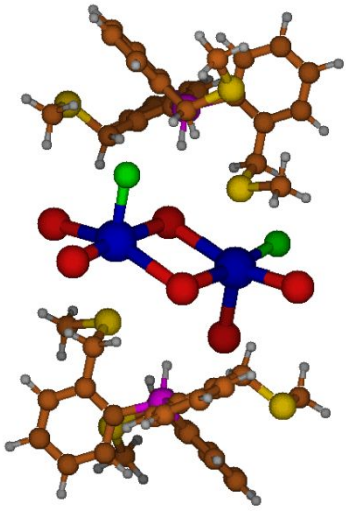
Excited State 19: Singlet-A 3.7556 eV 330.13 nm f=0.0011 <S**2>=0.000
357 -> 368 -0.20202
358 -> 367 0.44600
358 -> 369 0.46057
358 -> 370 -0.11386

Excited State 20: Singlet-A 3.7603 eV 329.72 nm f=0.0092 <S**2>=0.000
357 -> 369 -0.25367
358 -> 368 0.51682
358 -> 369 -0.20529
358 -> 370 -0.31756

Table S4: Relative energies of $[HPS_3BiCl_3Br]_2$ at ωB97XD/ def2-SVP (PCM)

Letter	Isomer (Br)	Energy (kcal/mol)
a		0,00
b		-1,69
c		-1,06

d		-0,52
e		-0,77
f		-3,06

g		-1,53
h		-2,45
i		-1,89

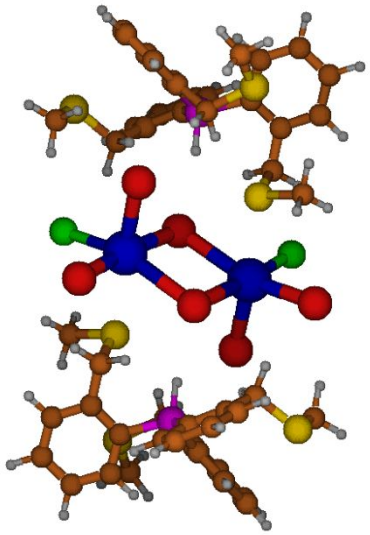
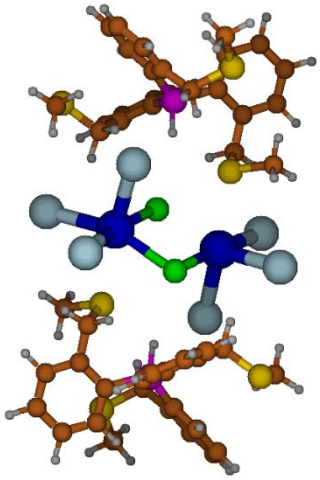
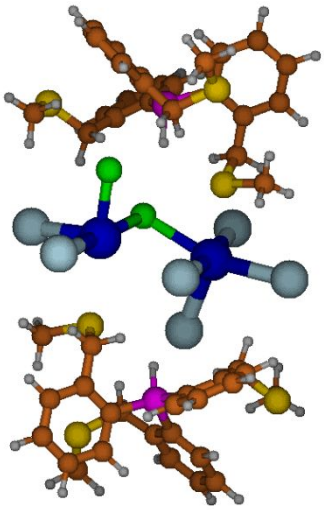
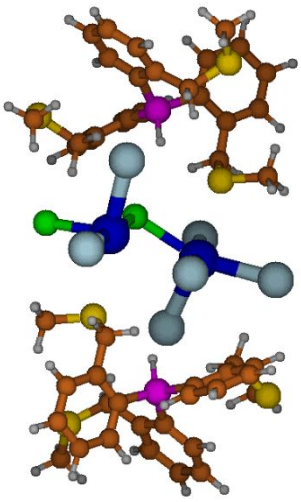
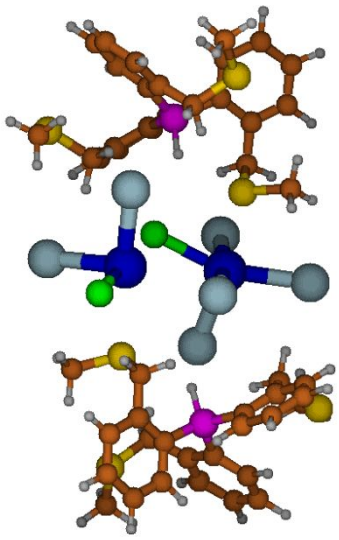
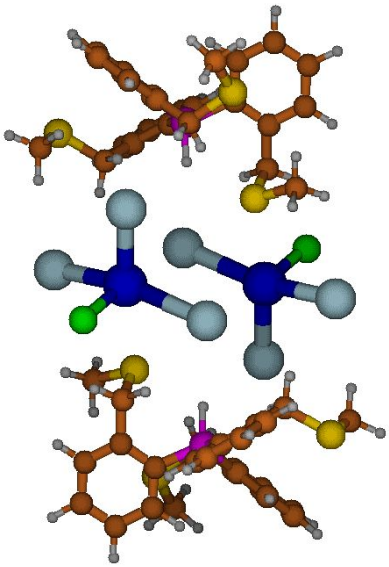
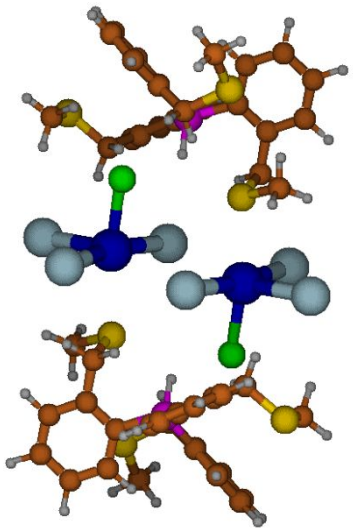
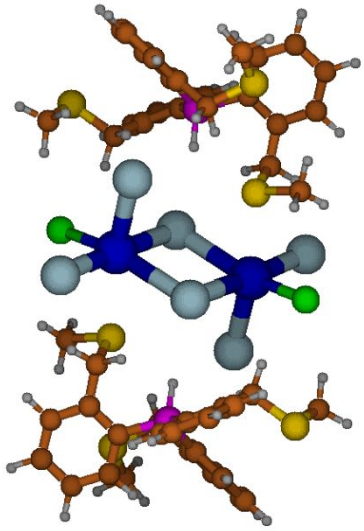
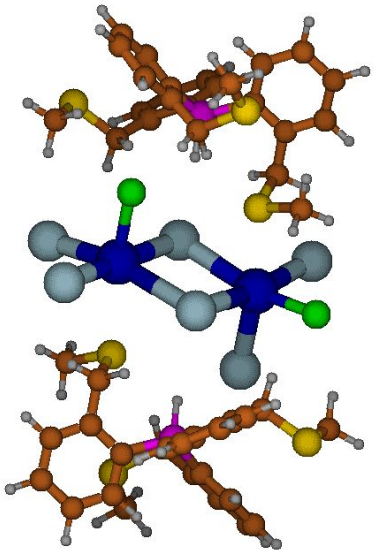
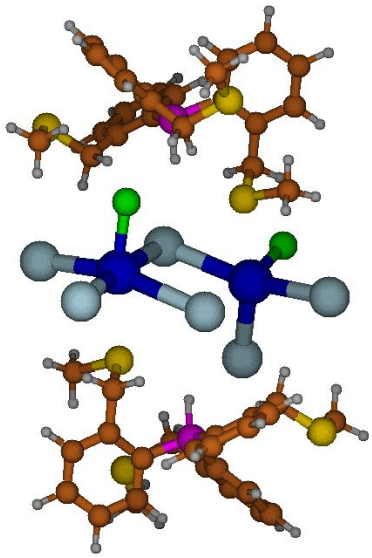
j		-1,16

Table S5: Relative energies of $[HPS_3BiCl_3I]_2$ at ωB97XD/ def2-SVP (PCM)

Letter	Isomer (I)	Energy (kcal/mol)
a		6,93
b		2,09
c		4,37

d		4,06
e		4,06
f		0,00

g		4,47
h		1,64
i		2,07

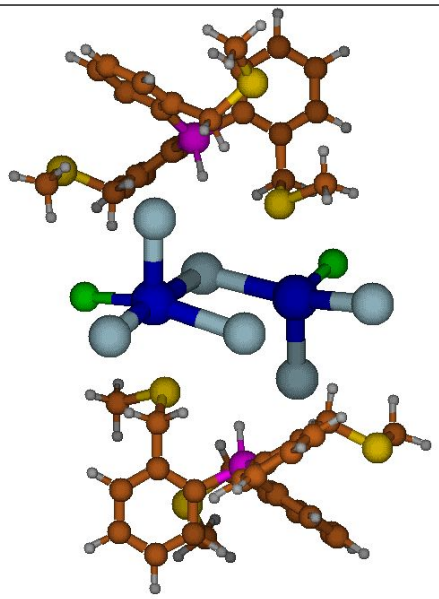
j		4,09

Table S6: Wiberg bond indices in $[Ag(PS_3)]_2^{2+}$ at the ωB97XD/ def2-SVP (PCM) level.

	Wiberg bond index with Ag	Bond distance
S3'	0,2674	2,591
S1	0,2683	2,657
S2	0,2519	2,679
S3	0,0727	3,484
P	0,3023	2,519

Total energies (E; in a.u.) and XYZ coordinates (in Å)

$BiCl_3$ ωB97XD/aug-cc-pVDZ(-PP) (PCM)

E= -1595.465623

Bi	-0.043457	0.052163	-0.037139
Cl	0.022857	-0.026802	2.448955
Cl	2.422093	-0.027352	-0.357118
Cl	-0.417543	-2.386499	-0.357767

$[BiCl_4]^-$ ωB97XD/aug-cc-pVDZ(-PP) (PCM)

E= -2055.875437

Bi	-0.225486	-0.418127	0.276671
Cl	0.449676	0.352665	2.775287
Cl	2.103141	-0.024176	-0.606852
Cl	-1.068195	-1.505592	-2.047496
Cl	-1.138705	1.857254	-0.312688

PS_3 ωB97XD/cc-pVDZ(-PP) (PCM)

E=-2466.5129017

C	-2.826834	-0.706568	-0.234774
C	-2.032292	0.428227	0.042545
C	-2.652516	1.674058	0.183858
C	-4.034237	1.809555	0.049017
C	-4.815986	0.691198	-0.222537
C	-4.210307	-0.556370	-0.358891
P	-0.201223	0.204202	0.116719
C	0.399804	1.945750	0.265829
C	0.732449	2.637314	-0.918633
C	1.227024	3.941397	-0.829422
C	1.404091	4.562917	0.405274
C	1.078696	3.880396	1.573526
C	0.577188	2.581543	1.499037
C	0.606739	1.986337	-2.273404
S	2.104919	0.997466	-2.647276
C	1.354249	-0.391281	-3.530306
C	-2.215039	-2.069592	-0.439036
S	-1.787563	-2.301090	-2.202068
C	-0.486546	-3.546127	-2.027392
C	0.043485	-0.414903	1.839506
C	1.327461	-0.875581	2.200894
C	1.528139	-1.398398	3.482016
C	0.486053	-1.473218	4.402930
C	-0.780433	-1.017474	4.047450
C	-0.995152	-0.489879	2.775198
C	2.482466	-0.855279	1.231790
S	2.584142	-2.459184	0.362851
C	3.853442	-2.030126	-0.852148
H	1.485726	4.475188	-1.747677
H	1.799818	5.579744	0.452059
H	1.213017	4.356801	2.547001
H	0.320691	2.052589	2.419623
H	2.522786	-1.760814	3.755362
H	0.664346	-1.889678	5.396715
H	-1.605275	-1.066740	4.761724
H	-1.990050	-0.128077	2.506046
H	-2.048462	2.556572	0.404564

H	-4.496803	2.792440	0.161114
H	-5.898333	0.787570	-0.330932
H	-4.821207	-1.436806	-0.575454
H	3.426914	-0.680540	1.769691
H	2.377267	-0.064429	0.473802
H	0.469825	2.749991	-3.052895
H	-0.257361	1.307569	-2.317537
H	-1.294819	-2.195719	0.149221
H	-2.918661	-2.854935	-0.124698
H	-0.114798	-3.765466	-3.037865
H	0.341600	-3.157338	-1.414049
H	-0.875081	-4.475841	-1.586764
H	3.936179	-2.870726	-1.554688
H	3.558446	-1.124797	-1.402807
H	4.830113	-1.869055	-0.371590
H	2.149832	-1.129724	-3.702492
H	0.563161	-0.847595	-2.915998
H	0.943858	-0.081669	-4.502321

[HPS_3]$^+$ ωB97XD/cc-pVDZ(-PP) (PCM)

E= -2466.952320

C	0.811742	2.726834	-0.111345
C	1.370694	1.492481	-0.498527
C	2.552346	1.433814	-1.245922
C	3.195399	2.610970	-1.616542
C	2.653870	3.838165	-1.241191
C	1.472902	3.892161	-0.502510
P	0.604326	-0.055032	0.028225
C	1.107595	-1.404743	-1.060756
C	0.493039	-1.566443	-2.318572
C	0.953757	-2.594274	-3.142622
C	1.996855	-3.427503	-2.741059
C	2.594980	-3.256803	-1.494687
C	2.149324	-2.244073	-0.650409
C	-0.679471	-0.727770	-2.754839
S	-2.197008	-1.460898	-2.035072
C	-3.430389	-0.246861	-2.574894
C	-0.494045	2.820979	0.633642
S	-1.856547	2.708414	-0.586726
C	-3.285767	2.738203	0.528764
C	1.055341	-0.425736	1.736731
C	2.226551	0.136049	2.257547
C	2.627091	-0.178250	3.552768
C	1.855076	-1.047284	4.320271
C	0.685373	-1.598956	3.799996
C	0.265264	-1.307206	2.501315
C	-1.034877	-1.870854	1.990868
S	-2.350878	-0.630859	2.289835
C	-3.762746	-1.476996	1.529363
H	-0.799255	0.087595	-0.047674
H	0.080575	-2.267987	4.414722
H	0.482094	-2.744242	-4.115345
H	1.050921	4.859123	-0.223393
H	2.160950	-1.294762	5.337589

H	2.339937	-4.219754	-3.407721
H	3.152134	4.764905	-1.528591
H	3.538905	0.258612	3.960283
H	3.406424	-3.911033	-1.175472
H	4.116810	2.566000	-2.197327
H	2.826481	0.820097	1.654927
H	2.613712	-2.110551	0.328105
H	2.972730	0.470884	-1.540663
H	-1.001979	-2.106473	0.914978
H	-0.596131	0.321280	-2.428059
H	-0.614120	2.020943	1.382050
H	-1.284573	-2.799007	2.522527
H	-0.762396	-0.725499	-3.849952
H	-0.563395	3.780273	1.163887
H	-3.558824	-1.684179	0.470671
H	-3.166267	0.753338	-2.207176
H	-3.230051	1.906234	1.243335
H	-3.992086	-2.408087	2.064789
H	-3.521786	-0.242263	-3.669278
H	-3.342765	3.697516	1.060294
H	-4.617562	-0.792838	1.609889
H	-4.386231	-0.557579	-2.133032
H	-4.177630	2.621002	-0.100677

PS_3BiCl_3 ωB97XD/cc-pVDZ(-PP) (PCM)

E= -4062.012637

C	-2.879300	-0.119106	-2.470799
C	-2.178819	0.679293	-1.558089
C	-1.841426	2.003558	-1.925855
C	-2.211375	2.463958	-3.194053
C	-2.891338	1.653136	-4.099925
C	-3.230961	0.356177	-3.733004
P	-1.578973	-0.063120	0.027690
C	-2.389864	0.949861	1.342450
C	-1.857033	0.948137	2.645768
C	-2.454621	1.753839	3.622623
C	-3.567085	2.536614	3.331354
C	-4.109083	2.517948	2.047236
C	-3.522498	1.727472	1.063902
C	-0.673515	0.100703	3.044602
S	0.908376	1.002343	2.777834
C	2.007482	0.039201	3.857219
C	-1.142290	2.976988	-1.011021
S	0.662794	2.766572	-0.809226
C	1.228829	2.967403	-2.518827
C	-2.524852	-1.652776	0.143044
C	-3.727751	-1.729539	0.857267
C	-4.424940	-2.930361	0.964464
C	-3.926018	-4.077279	0.352796
C	-2.732448	-4.012655	-0.360049
C	-2.019505	-2.814702	-0.475403
C	-0.723163	-2.825528	-1.243788
S	0.692379	-2.961147	-0.082446
C	1.896527	-3.814167	-1.138786

Bi	1.876765	-0.017905	-0.022005
Cl	3.649046	-1.610966	1.064955
Cl	3.753402	1.786495	0.019272
Cl	2.165457	-0.517160	-2.559459
H	2.050983	-3.248905	-2.066872
H	1.541320	-4.831794	-1.348297
H	2.834414	-3.848601	-0.570847
H	1.991279	-1.023224	3.581919
H	1.704810	0.178285	4.903432
H	3.019723	0.435193	3.705742
H	2.317807	2.832873	-2.497521
H	0.983217	3.978880	-2.870266
H	0.778441	2.206491	-3.169565
H	-0.586401	-1.934016	-1.873853
H	-0.684704	-3.704572	-1.900734
H	-0.642406	-0.858788	2.509849
H	-0.722756	-0.118857	4.119903
H	-1.531184	2.943577	0.014535
H	-1.294258	4.002235	-1.376609
H	-4.132906	-0.840159	1.339777
H	-5.360510	-2.964506	1.524732
H	-4.463253	-5.023776	0.429934
H	-2.337836	-4.911620	-0.838301
H	-3.947228	1.717478	0.058181
H	-4.989213	3.117133	1.809093
H	-4.014629	3.156163	4.109867
H	-2.036570	1.761503	4.631585
H	-3.165419	-1.134734	-2.195752
H	-3.776764	-0.291134	-4.420891
H	-3.160078	2.041593	-5.083299
H	-1.963660	3.490623	-3.473057

$[HPS_3]^+[BiCl_4]^-$ ωB97XD/cc-pVDZ(-PP) (PCM)

E= -4522.830080

C	2.608474	-0.394829	2.210197
C	2.882860	0.323837	1.023803
C	3.943446	1.234367	0.960086
C	4.756689	1.444791	2.069925
C	4.495391	0.752313	3.246846
C	3.434462	-0.150824	3.310511
P	1.893234	0.111099	-0.474186
C	2.029867	1.541894	-1.571486
C	1.476129	2.785025	-1.205852
C	1.564808	3.830938	-2.127640
C	2.188389	3.660210	-3.360967
C	2.738170	2.427892	-3.706787
C	2.653221	1.365441	-2.813419
C	0.815866	3.038543	0.122364
S	1.918090	4.044840	1.195292
C	1.456149	3.371211	2.815606
C	1.494301	-1.400298	2.358443
S	1.850417	-3.049977	1.648765
C	3.335307	-3.504720	2.585377
C	2.383089	-1.391315	-1.355728

C	3.726738	-1.768434	-1.275491
C	4.170195	-2.912309	-1.931262
C	3.264305	-3.679397	-2.658810
C	1.924955	-3.299883	-2.737820
C	1.456763	-2.151240	-2.095983
C	-0.003957	-1.794982	-2.179380
S	-0.902818	-2.176729	-0.630568
C	-1.139665	-3.965446	-0.748153
Cl	-1.579104	0.593470	1.769564
Bi	-3.199726	-0.019148	-0.098229
Cl	-4.343491	-1.894443	1.415360
Cl	-1.635430	1.380004	-1.839457
Cl	-4.817990	1.885589	0.452453
H	0.545114	-0.005048	-0.084197
H	-1.691456	-4.222057	-1.661759
H	-0.164866	-4.470674	-0.721072
H	-1.726154	-4.252524	0.134024
H	3.608434	-4.516742	2.257221
H	4.168581	-2.821311	2.368033
H	3.133331	-3.520226	3.666051
H	1.224685	-3.907237	-3.314196
H	3.599283	-4.582751	-3.170382
H	5.218422	-3.204232	-1.864831
H	4.430213	-1.176774	-0.686895
H	-0.175830	-0.719997	-2.347230
H	-0.491392	-2.330363	-3.005342
H	3.234371	-0.679429	4.244272
H	5.115470	0.916910	4.129162
H	5.576344	2.161040	2.013813
H	4.127952	1.796357	0.043850
H	1.256304	-1.521358	3.424432
H	0.567745	-1.077753	1.862506
H	1.710242	2.302515	2.873642
H	2.039622	3.922203	3.565307
H	0.385220	3.516840	3.012170
H	1.125949	4.797330	-1.872344
H	2.237564	4.495732	-4.060748
H	3.223310	2.287046	-4.672826
H	3.067256	0.394983	-3.089246
H	-0.138493	3.561330	-0.028600
H	0.577073	2.113619	0.664243

[HPS_3BiCl_4]$_2$ ωB97XD/cc-pVDZ(-PP) (PCM)

E= -9045.714577

C	-8.451472	-0.758253	-1.013454
C	-7.243863	-1.137859	-0.418112
C	-6.977404	-2.489817	-0.113106
C	-7.970416	-3.424269	-0.415048
C	-9.179461	-3.047542	-0.999566
C	-9.423998	-1.712323	-1.301779
P	-6.048839	0.173914	-0.062399
C	-6.126676	1.500778	-1.296801
C	-5.295010	1.534655	-2.435242
C	-5.464265	2.596186	-3.327921

C	-6.409596	3.595108	-3.107569
C	-7.212852	3.560621	-1.971522
C	-7.065136	2.516502	-1.064653
C	-4.216112	0.522054	-2.724539
S	-4.774371	-1.212767	-2.796800
C	-6.163332	-1.083873	-3.954409
C	-5.683653	-2.978150	0.490998
S	-5.323577	-2.325551	2.158349
C	-6.847444	-2.780398	3.028455
C	-6.362651	0.918451	1.563753
C	-5.394997	1.757380	2.156428
C	-5.670452	2.275276	3.423404
C	-6.868377	1.992468	4.079333
C	-7.822205	1.180259	3.474283
C	-7.566481	0.640882	2.215567
C	-4.087281	2.109077	1.494474
S	-2.916600	0.704546	1.380557
C	-2.558137	0.394626	3.125598
Bi	-0.483590	2.102202	0.126459
Cl	-2.217861	3.441684	-1.345761
Cl	-0.777516	-0.117706	-1.776346
Bi	0.484447	-2.105760	-0.122595
Cl	0.776867	0.113117	1.781276
Cl	2.221062	-3.444682	1.347760
Cl	0.689047	-3.768075	-2.136699
Cl	-1.749095	-3.035062	0.875509
Cl	-0.688717	3.765138	2.139745
Cl	1.750084	3.032539	-0.870837
S	2.915390	-0.705826	-1.379591
C	2.555352	-0.395801	-3.124319
C	4.087139	-2.109444	-1.494796
C	5.394036	-1.756739	-2.157880
C	6.361446	-0.916686	-1.566344
C	7.564525	-0.638457	-2.219240
C	7.819770	-1.178223	-3.477882
C	6.866205	-1.991589	-4.081784
C	5.669033	-2.275091	-3.424782
P	6.048417	-0.171447	0.059685
C	7.243313	1.140776	0.414268
C	6.976483	2.492554	0.108837
C	7.969488	3.427314	0.409856
C	9.178888	3.051069	0.993940
C	9.423781	1.716023	1.296649
C	8.451281	0.761661	1.009220
C	5.682316	2.980406	-0.494731
S	5.321142	2.326656	-2.161373
C	6.843931	2.782029	-3.033104
C	6.127618	-1.497630	1.294722
C	7.066598	-2.512941	1.062882
C	7.215439	-3.556208	1.970552
C	6.412854	-3.590221	3.107094
C	5.466959	-2.591754	3.327094
C	5.296504	-1.531150	2.433566

C	4.216881	-0.519148	2.722246
S	4.774101	1.216046	2.794141
C	6.163311	1.088354	3.951577
H	4.749045	0.354962	0.032781
H	2.097860	-1.286454	-3.575263
H	3.481683	-0.113639	-3.642090
H	1.845203	0.440099	-3.139705
H	6.730721	2.419867	-4.063642
H	7.723607	2.302836	-2.579941
H	6.976782	3.873121	-3.044254
H	4.929014	-2.919482	-3.903039
H	7.051330	-2.414554	-5.070083
H	8.760594	-0.956388	-3.982243
H	8.307197	0.007995	-1.749218
H	4.219294	-2.454794	-0.457435
H	3.583421	-2.923439	-2.034790
H	7.785131	4.479529	0.185887
H	9.930057	3.810535	1.215104
H	10.362889	1.411760	1.759093
H	8.638410	-0.284036	1.258984
H	5.687745	4.078150	-0.531761
H	4.817076	2.685482	0.120707
H	5.820305	0.729358	4.931931
H	6.574040	2.101255	4.057771
H	6.946567	0.423624	3.559316
H	4.831018	-2.638064	4.212503
H	6.515386	-4.402955	3.827478
H	7.951780	-4.338028	1.783622
H	7.682467	-2.497251	0.161510
H	3.716793	-0.777435	3.665012
H	3.433032	-0.534303	1.948375
H	-4.749828	-0.353309	-0.034900
H	-2.103727	1.286368	3.577519
H	-3.484239	0.109539	3.642145
H	-1.845410	-0.439048	3.141208
H	-6.734681	-2.419386	4.059444
H	-7.726343	-2.299971	2.575100
H	-6.981276	-3.871384	3.038435
H	-4.930211	2.918718	3.902588
H	-7.053892	2.415070	5.067714
H	-8.763607	0.959024	3.977827
H	-8.309289	-0.004790	1.744691
H	-4.218035	2.454407	0.456928
H	-3.583496	2.922786	2.034863
H	-7.786363	-4.476618	-0.191462
H	-9.930646	-3.806781	-1.221449
H	-10.362847	-1.407694	-1.764510
H	-8.638295	0.287609	-1.262781
H	-5.689204	-4.075916	0.527324
H	-4.817991	-2.682953	-0.123709
H	-5.819798	-0.725221	-4.934706
H	-6.575022	-2.096378	-4.060661
H	-6.946003	-0.418361	-3.562296

H	-4.827852	2.642797	-4.212977
H	-6.511186	4.408522	-3.827319
H	-7.948830	4.342720	-1.784339
H	-7.681467	2.500459	-0.163615
H	-3.716281	0.780293	-3.667469
H	-3.431896	0.536541	-1.951039

[Ag(PS_3)]$^+$ ωB97XD/def2-SVP (PCM)

E= -2612.225881

C	2.331295	1.166202	0.954865
C	1.209627	0.421299	1.400856
C	1.305172	-0.282350	2.606743
C	2.464366	-0.244003	3.382229
C	3.551028	0.513784	2.963365
C	3.475378	1.210060	1.758405
P	-0.291612	0.309943	0.321694
Ag	1.105162	-0.975402	-1.471262
S	2.819654	0.847901	-1.814163
C	4.435035	0.195412	-1.328384
C	2.379448	1.895205	-0.365677
C	-1.470755	-0.704757	1.305372
C	-1.889723	-1.984046	0.871807
C	-2.692804	-2.747954	1.730309
C	-3.113600	-2.266504	2.966212
C	-2.745853	-0.984972	3.365229
C	-1.930185	-0.219861	2.537610
C	-1.645125	-2.556950	-0.504105
S	0.026420	-3.197340	-0.921174
C	0.666066	-3.756071	0.676569
C	-0.944306	2.030366	0.381903
C	-1.624931	2.573061	-0.729600
C	-2.118156	3.880386	-0.643218
C	-1.925690	4.654346	0.497975
C	-1.219488	4.130961	1.578337
C	-0.729460	2.829731	1.513654
C	-1.825281	1.805238	-2.010567
S	-3.134467	0.550875	-1.818708
C	-2.978398	-0.272232	-3.421635
H	5.152751	1.020648	-1.231764
H	4.370164	-0.367754	-0.388942
H	4.755255	-0.474510	-2.136257
H	1.675350	-4.143298	0.488230
H	0.716434	-2.930498	1.397594
H	0.032065	-4.563202	1.065535
H	4.332187	1.801965	1.426747
H	4.459733	0.563902	3.566012
H	2.505282	-0.801308	4.319964
H	0.460465	-0.872349	2.963489
H	1.420276	2.351159	-0.645521
H	3.122039	2.704103	-0.331555
H	-3.016541	-3.739744	1.405932
H	-3.744025	-2.887130	3.605802
H	-3.087846	-0.578337	4.318650
H	-1.638835	0.778141	2.868647

H	-2.342422	-3.387362	-0.671354
H	-1.849440	-1.790285	-1.263976
H	-1.977954	-0.713650	-3.546590
H	-3.727761	-1.074406	-3.448005
H	-3.177119	0.427229	-4.245574
H	-2.653105	4.301159	-1.497845
H	-2.318870	5.672128	0.537088
H	-1.045755	4.733125	2.472008
H	-0.157559	2.436303	2.357235
H	-2.105469	2.493814	-2.820157
H	-0.895440	1.293840	-2.306286

$[Ag(PS_3)]_2^{2+}$ ωB97XD/ def2-SVP (PCM)

E=-5224.512738

C	6.064106	-1.911819	2.727661
C	5.398812	-1.446340	1.587972
C	4.866832	-0.131901	1.608730
C	5.004243	0.641268	2.768233
C	5.655260	0.147099	3.897061
C	6.192160	-1.134130	3.876227
C	5.312264	-2.389052	0.411809
S	3.717290	-3.269136	0.197961
C	3.481331	-3.990302	1.839291
P	3.881889	0.525216	0.203159
C	5.039691	0.586319	-1.226046
C	4.542608	0.751254	-2.537705
C	5.456193	0.792837	-3.597583
C	6.827259	0.673828	-3.386665
C	7.313508	0.519472	-2.092172
C	6.421865	0.481516	-1.022967
C	3.078612	0.900845	-2.866707
S	2.096595	-0.651355	-2.902707
C	3.162418	-1.761066	-3.852162
Ag	2.127093	-1.199384	-0.290096
S	-0.296732	-1.791834	0.405042
C	-0.150877	-3.490045	1.011278
C	-1.153906	-2.021473	-1.205135
C	-2.420900	-2.826026	-1.080003
C	-2.354791	-4.182576	-1.423572
C	-3.453293	-5.026263	-1.286680
C	-4.650509	-4.519504	-0.790707
C	-4.738141	-3.172030	-0.454021
C	-3.642337	-2.309166	-0.596329
P	-3.881892	-0.525202	-0.203178
C	-5.039717	-0.586309	1.226007
C	-4.542657	-0.751292	2.537670
C	-5.456258	-0.792857	3.597535
C	-6.827315	-0.673782	3.386601
C	-7.313540	-0.519379	2.092104
C	-6.421881	-0.481441	1.022912
C	-3.078671	-0.900956	2.866689
S	-2.096560	0.651185	2.902740
C	-3.162302	1.760922	3.852258
C	-4.866829	0.131977	-1.608724

C	-5.398825	1.446408	-1.587876
C	-6.064136	1.911953	-2.727529
C	-6.192190	1.134294	-3.876166
C	-5.655266	-0.146925	-3.897049
C	-5.004245	-0.641128	-2.768237
C	-5.312264	2.389027	-0.411640
S	-3.717288	3.269110	-0.197788
Ag	-2.127091	1.199339	0.290101
S	0.296728	1.791785	-0.405067
C	0.150860	3.489979	-1.011345
C	-3.481386	3.990376	-1.839084
C	3.642339	2.309196	0.596235
C	2.420940	2.826063	1.079915
C	2.354837	4.182630	1.423424
C	3.453336	5.026310	1.286476
C	4.650543	4.519530	0.790508
C	4.738170	3.172040	0.453881
C	1.153952	2.021511	1.205104
H	4.130832	-1.909681	-3.357024
H	3.313156	-1.369154	-4.867015
H	2.636333	-2.722421	-3.916171
H	3.358431	-3.216066	2.608309
H	4.336683	-4.633477	2.087554
H	2.580938	-4.615545	1.788536
H	-0.435548	4.113177	-0.322563
H	-0.363491	3.423721	-1.978997
H	1.146653	3.928012	-1.160625
H	2.965561	1.377055	-3.850399
H	2.543104	1.525643	-2.137134
H	6.087440	-3.162958	0.498469
H	5.470508	-1.889064	-0.552988
H	0.456251	2.509051	1.899153
H	1.319165	0.998723	1.570240
H	6.812412	0.363896	-0.009170
H	8.386096	0.433202	-1.909934
H	7.514546	0.708591	-4.233854
H	5.081808	0.929814	-4.615253
H	4.600472	1.654355	2.798140
H	5.749195	0.773119	4.786112
H	6.716344	-1.530641	4.747458
H	6.502721	-2.912759	2.711129
H	5.685589	2.783777	0.075907
H	5.520072	5.168095	0.671214
H	3.370585	6.078613	1.564410
H	1.416567	4.587398	1.811340
H	-4.130717	1.909609	3.357145
H	-3.313057	1.368971	4.867094
H	-2.636154	2.722240	3.916308
H	-3.358491	3.216188	-2.608150
H	-4.336755	4.633550	-2.087287
H	-2.581003	4.615633	-1.788315
H	0.435531	-4.113229	0.322485
H	0.363469	-3.423815	1.978935

H	-1.146683	-3.928054	1.160552
H	-2.965657	-1.377200	3.850368
H	-2.543197	-1.525765	2.137102
H	-6.087439	3.162941	-0.498220
H	-5.470484	1.888987	0.553136
H	-0.456196	-2.508984	-1.899194
H	-1.319127	-0.998671	-1.570230
H	-6.812410	-0.363784	0.009112
H	-8.386122	-0.433059	1.909855
H	-7.514616	-0.708532	4.233782
H	-5.081892	-0.929871	4.615208
H	-4.600470	-1.654210	-2.798192
H	-5.749187	-0.772903	-4.786132
H	-6.716382	1.530827	-4.747382
H	-6.502762	2.912887	-2.710928
H	-5.685574	-2.783799	-0.076051
H	-5.520040	-5.168075	-0.671457
H	-3.370537	-6.078553	-1.564661
H	-1.416516	-4.587345	-1.811474

$[HPS_3BiCl_3Br]_2$ ('a' isomer) ωB97XD/ def2-SVP (PCM)

E= -21725.252207

C	7.227914	1.479336	-0.432944
C	6.351053	0.668567	0.294738
C	6.295332	0.728875	1.706698
C	7.106250	1.675164	2.339209
C	7.972323	2.494116	1.614458
C	8.048649	2.388026	0.229378
P	5.254002	-0.433448	-0.610248
C	5.198681	-0.089402	-2.379331
C	4.615251	1.099802	-2.860811
C	4.520614	1.265886	-4.246170
C	4.998246	0.298393	-5.125510
C	5.583733	-0.868545	-4.637343
C	5.679014	-1.065419	-3.264506
C	4.119335	2.195623	-1.960937
S	5.198042	3.667568	-2.103878
C	4.954591	4.387887	-0.462707
C	5.436103	-0.181762	2.548517
S	6.265760	-1.708754	3.109719
C	7.439705	-1.058579	4.319969
C	5.757371	-2.140572	-0.344703
C	4.818817	-3.189888	-0.361974
C	5.289723	-4.491007	-0.169042
C	6.648449	-4.746655	0.012025
C	7.568416	-3.701951	0.004554
C	7.120657	-2.395759	-0.165576
C	3.350722	-2.957064	-0.581544
S	2.472009	-2.328744	0.892022
C	2.602992	-3.737244	2.011709
Bi	-0.400096	-2.129254	-0.401283
Br	0.452130	-3.828018	-2.411434
Br	-1.044495	-4.214898	1.292099

Br	-2.832674	-1.898331	-1.667968
Cl	-1.299650	-0.056580	1.462560
Cl	1.299735	0.056880	-1.462431
Bi	0.400006	2.129442	0.401305
Br	2.832432	1.898528	1.668305
Br	-0.452957	3.828348	2.411163
Br	1.044733	4.215226	-1.291814
S	-2.471639	2.327924	-0.893014
C	-2.602775	3.735910	-2.013329
C	-3.350374	2.956910	0.580267
C	-4.818466	3.189710	0.360687
C	-5.757072	2.140427	0.344091
C	-7.120389	2.395601	0.165171
C	-7.568128	3.701735	-0.005457
C	-6.648107	4.746385	-0.013668
C	-5.289352	4.490757	0.167220
P	-5.253735	0.433364	0.610129
C	-6.351101	-0.668867	-0.294210
C	-6.295834	-0.729513	-1.706176
C	-7.106880	-1.676025	-2.338192
C	-7.972685	-2.494840	-1.612967
C	-8.048590	-2.388392	-0.227890
C	-7.227689	-1.479496	0.433944
C	-5.436919	0.180958	-2.548497
S	-6.266933	1.707613	-3.110097
C	-7.440696	1.056888	-4.320230
C	-5.198048	0.089912	2.379327
C	-5.678136	1.066280	3.264249
C	-5.582652	0.869882	4.637142
C	-4.997214	-0.296949	5.125620
C	-4.519812	-1.264785	4.246534
C	-4.614639	-1.099175	2.861132
C	-4.118883	-2.195348	1.961607
S	-5.197657	-3.667187	2.105013
C	-4.953995	-4.388103	0.464133
H	-3.951518	0.248876	0.106076
H	-2.132383	4.625100	-1.572658
H	-3.656373	3.924956	-2.260721
H	-2.059675	3.457133	-2.925222
H	-7.920889	1.928547	-4.785088
H	-8.217237	0.441333	-3.844695
H	-6.927788	0.476234	-5.100532
H	-4.577019	5.318573	0.172282
H	-6.988199	5.773586	-0.158128
H	-8.632050	3.897608	-0.145456
H	-7.837069	1.571723	0.147905
H	-3.149614	2.205145	1.359950
H	-2.855200	3.878959	0.911346
H	-7.051146	-1.780014	-3.423768
H	-8.590929	-3.223879	-2.140321
H	-8.722814	-3.026559	0.344838
H	-7.252986	-1.422602	1.523206
H	-5.067910	-0.361936	-3.430547

H	-4.542652	0.537447	-2.017686
H	-5.348319	-3.719711	-0.315791
H	-5.510979	-5.334648	0.446577
H	-3.889109	-4.586287	0.280567
H	-4.058403	-2.174016	4.638722
H	-4.905056	-0.453155	6.202105
H	-5.955446	1.632403	5.322515
H	-6.119553	1.987896	2.880836
H	-3.087164	-2.465599	2.227394
H	-4.096171	-1.904618	0.901856
H	3.951652	-0.249223	-0.106464
H	2.132611	-4.626210	1.570579
H	3.656556	-3.926414	2.259154
H	2.059776	-3.458858	2.923653
H	7.919964	-1.930445	4.784370
H	8.216178	-0.442814	3.844595
H	6.926905	-0.478278	5.100602
H	4.577422	-5.318847	-0.174621
H	6.988567	-5.773905	0.156075
H	8.632313	-3.897839	0.144731
H	7.837293	-1.571854	-0.147757
H	3.149932	-2.204951	-1.360882
H	2.855667	-3.879024	-0.913053
H	7.050208	1.778864	3.424797
H	8.590457	3.222970	2.142196
H	8.723088	3.026306	-0.342972
H	7.253567	1.422683	-1.522210
H	5.067001	0.360880	3.430685
H	4.541889	-0.537937	2.017410
H	5.348553	3.718988	0.316966
H	5.511999	5.334175	-0.444705
H	3.889783	4.586475	-0.279138
H	4.059184	2.175210	-4.638116
H	4.906233	0.454951	-6.201957
H	5.956721	-1.630788	-5.322922
H	6.120458	-1.987129	-2.881349
H	3.087595	2.465840	-2.226668
H	4.096686	1.904508	-0.901288

[$HPS_3BiCl_3Br]_2$ ('b' isomer) ωB97XD/ def2-SVP (PCM)

E= -21725.254906

C	7.282689	1.502537	-0.159918
C	6.334048	0.717323	0.503094
C	6.160098	0.803308	1.903794
C	6.934320	1.744035	2.588327
C	7.873296	2.536249	1.927647
C	8.061775	2.407801	0.555301
P	5.304699	-0.385828	-0.477215
C	5.408673	-0.053794	-2.247116
C	4.873116	1.133698	-2.785408
C	4.913757	1.296852	-4.173936
C	5.476452	0.329314	-5.001202
C	6.012415	-0.836255	-4.456238
C	5.972969	-1.030763	-3.080360

C	4.290609	2.231327	-1.940835
S	5.369140	3.710901	-1.993962
C	5.012879	4.419060	-0.368243
C	5.214486	-0.073612	2.686196
S	5.951728	-1.622964	3.310837
C	7.093094	-0.999617	4.565134
C	5.776998	-2.094532	-0.161323
C	4.839579	-3.142399	-0.231606
C	5.292571	-4.443028	0.003379
C	6.635278	-4.700961	0.275710
C	7.556211	-3.658022	0.322109
C	7.124086	-2.352440	0.112148
C	3.387501	-2.909443	-0.538187
S	2.436651	-2.252007	0.877083
C	2.525931	-3.625472	2.042717
Bi	-0.323273	-2.106291	-0.539224
Br	0.583816	-3.671543	-2.625314
Br	-1.013277	-4.307896	0.979693
Br	-2.757201	-1.712642	-1.785193
Br	-1.049811	-0.141164	1.716167
Cl	1.405409	0.094035	-1.505158
Bi	0.577326	2.170747	0.371705
Cl	2.933416	1.974948	1.439257
Br	-0.164280	3.929501	2.369304
Br	1.138436	4.200102	-1.408510
S	-2.393052	2.360991	-0.722737
C	-2.573466	3.803556	-1.791625
C	-3.239990	2.926884	0.794436
C	-4.706436	3.196137	0.601575
C	-5.665723	2.168828	0.505274
C	-7.022580	2.464395	0.338724
C	-7.444894	3.788072	0.265106
C	-6.505306	4.811990	0.340625
C	-5.152504	4.516473	0.504968
P	-5.202047	0.435138	0.644597
C	-6.306699	-0.578623	-0.349881
C	-6.240858	-0.529998	-1.761839
C	-7.051880	-1.419562	-2.471651
C	-7.929122	-2.285846	-1.819259
C	-8.016346	-2.285858	-0.430747
C	-7.194845	-1.437229	0.306155
C	-5.373587	0.439858	-2.525352
S	-6.202354	2.003609	-2.976970
C	-7.339802	1.449653	-4.266870
C	-5.168630	-0.049581	2.380818
C	-5.648527	0.859165	3.334941
C	-5.568732	0.554910	4.689003
C	-4.998895	-0.652337	5.089658
C	-4.523549	-1.554316	4.141913
C	-4.603698	-1.280405	2.772802
C	-4.107387	-2.306470	1.793512
S	-5.197632	-3.777237	1.805899
C	-4.929998	-4.367972	0.117880

H	-3.901873	0.268873	0.130407
H	-2.113051	4.687216	-1.329881
H	-3.635028	3.979532	-2.013668
H	-2.041410	3.566747	-2.721650
H	-7.809616	2.354635	-4.675202
H	-8.127456	0.797516	-3.863927
H	-6.803652	0.932760	-5.076032
H	-4.423977	5.327390	0.570846
H	-6.824161	5.853781	0.271788
H	-8.504080	4.013567	0.134201
H	-7.755093	1.658753	0.254243
H	-3.045159	2.134196	1.534078
H	-2.725640	3.823715	1.164194
H	-6.987399	-1.439470	-3.561484
H	-8.547871	-2.966957	-2.406642
H	-8.700675	-2.960626	0.085200
H	-7.231209	-1.464219	1.396192
H	-4.997730	-0.034405	-3.443339
H	-4.482826	0.755001	-1.963282
H	-5.314747	-3.641915	-0.613893
H	-5.484143	-5.311129	0.018833
H	-3.862252	-4.551255	-0.065025
H	-4.073932	-2.495746	4.465874
H	-4.917294	-0.891762	6.151649
H	-5.940269	1.266270	5.427973
H	-6.077000	1.812861	3.021597
H	-3.081266	-2.609478	2.046853
H	-4.071104	-1.930906	0.761010
H	3.966789	-0.185977	-0.087178
H	2.099860	-4.536006	1.600867
H	3.565837	-3.784376	2.359257
H	1.922045	-3.329809	2.910206
H	7.519660	-1.881342	5.062090
H	7.912159	-0.419462	4.117090
H	6.567543	-0.389018	5.313440
H	4.579123	-5.268759	-0.040597
H	6.961849	-5.727995	0.449384
H	8.608369	-3.854923	0.532337
H	7.840892	-1.530568	0.171385
H	3.231539	-2.168633	-1.338461
H	2.907013	-3.835899	-0.879290
H	6.790814	1.864327	3.664118
H	8.460197	3.261019	2.495184
H	8.793727	3.025008	0.032605
H	7.401413	1.425497	-1.241714
H	4.801950	0.488868	3.535843
H	4.348108	-0.401377	2.094908
H	5.361374	3.750206	0.432091
H	5.558700	5.370603	-0.311511
H	3.936843	4.605913	-0.250112
H	4.491387	2.204970	-4.610365
H	5.492461	0.485240	-6.081619
H	6.451530	-1.599372	-5.100444

H	6.376982	-1.951347	-2.655554
H	3.285657	2.493460	-2.301389
H	4.173016	1.949977	-0.885490

[$HPS_3BiCl_3Br]_2$ ('c' isomer) ωB97XD/def2-SVP (PCM)

E= -21725.253900

C	-7.206151	1.588980	0.549666
C	-6.357872	0.779413	-0.211899
C	-6.312605	0.884751	-1.621687
C	-7.111384	1.865354	-2.215767
C	-7.949817	2.682095	-1.457051
C	-8.010265	2.538579	-0.074557
P	-5.266915	-0.368070	0.643355
C	-5.197513	-0.117371	2.429051
C	-4.625023	1.050801	2.971722
C	-4.502496	1.132464	4.362513
C	-4.940663	0.102855	5.190168
C	-5.516314	-1.042245	4.642898
C	-5.639428	-1.155188	3.262874
C	-4.169131	2.210069	2.132029
S	-5.217581	3.670812	2.465236
C	-4.821489	4.645740	0.994215
C	-5.466450	-0.003202	-2.500798
S	-6.309826	-1.498717	-3.121819
C	-7.472481	-0.791176	-4.310618
C	-5.780970	-2.057594	0.293987
C	-4.850291	-3.112900	0.244868
C	-5.331653	-4.397862	-0.017650
C	-6.693741	-4.634051	-0.199905
C	-7.606309	-3.585717	-0.123475
C	-7.147565	-2.293976	0.114381
C	-3.380616	-2.903727	0.475355
S	-2.492558	-2.198124	-0.957514
C	-2.623269	-3.540706	-2.155395
Bi	0.334117	-2.088960	0.370322
Br	-0.529273	-3.799382	2.365157
Br	1.038168	-4.181293	-1.291961
Br	2.746545	-1.752517	1.667795
Br	1.118747	-0.002531	-1.740813
Cl	-1.359664	0.068148	1.468036
Bi	-0.513617	2.254180	-0.285047
Br	-2.978871	2.177204	-1.503678
Br	0.298274	4.193183	-2.083608
Cl	-1.053079	4.004977	1.553701
S	2.411470	2.354284	0.870404
C	2.499433	3.781675	1.971574
C	3.303493	2.977180	-0.597746
C	4.763206	3.239758	-0.353828
C	5.723023	2.210696	-0.297800
C	7.076509	2.497379	-0.093206
C	7.493762	3.815275	0.063326
C	6.552615	4.840434	0.032221
C	5.203692	4.553352	-0.173272
P	5.262380	0.488019	-0.538500

C	6.348429	-0.577743	0.421532
C	6.251564	-0.612228	1.832284
C	7.054454	-1.536412	2.506362
C	7.951751	-2.357894	1.823749
C	8.067840	-2.277060	0.439842
C	7.255822	-1.391977	-0.263906
C	5.359586	0.303647	2.633276
S	6.155226	1.853895	3.180306
C	7.312158	1.245109	4.427631
C	5.265595	0.097328	-2.298905
C	5.766533	1.054117	-3.193460
C	5.721155	0.818925	-4.562787
C	5.165080	-0.367285	-5.038695
C	4.667549	-1.316325	-4.150218
C	4.712709	-1.111882	-2.767593
C	4.193910	-2.185498	-1.853891
S	5.281420	-3.656615	-1.914278
C	4.971432	-4.328453	-0.264182
H	3.953434	0.291604	-0.057710
H	2.037692	4.658926	1.499593
H	3.543046	3.982380	2.249376
H	1.925185	3.515229	2.867729
H	7.770068	2.132835	4.884466
H	8.107325	0.631485	3.981335
H	6.791202	0.672937	5.208877
H	4.474957	5.366024	-0.207379
H	6.867709	5.876986	0.166088
H	8.550199	4.035193	0.222979
H	7.809071	1.688881	-0.043781
H	3.130163	2.213957	-1.373044
H	2.797296	3.886819	-0.946399
H	6.967445	-1.620010	3.591631
H	8.563190	-3.068002	2.383811
H	8.767076	-2.917106	-0.099808
H	7.314211	-1.355303	-1.352766
H	4.977669	-0.225228	3.518405
H	4.472693	0.635881	2.075004
H	5.340363	-3.639959	0.510764
H	5.520450	-5.277396	-0.197404
H	3.899166	-4.515900	-0.114781
H	4.228441	-2.240557	-4.532863
H	5.111913	-0.553211	-6.113117
H	6.109489	1.566786	-5.255675
H	6.185488	1.990804	-2.821410
H	3.173084	-2.472465	-2.144750
H	4.135588	-1.862739	-0.804989
H	-3.964257	-0.165310	0.147407
H	-2.162293	-4.456105	-1.760971
H	-3.676121	-3.708775	-2.420299
H	-2.071651	-3.213822	-3.046020
H	-7.956774	-1.639856	-4.812397
H	-8.246867	-0.189470	-3.814218
H	-6.951306	-0.183106	-5.064090

H	-4.625405	-5.229751	-0.063803
H	-7.042400	-5.649505	-0.397259
H	-8.672867	-3.766866	-0.263149
H	-7.858189	-1.465398	0.149168
H	-3.176237	-2.198729	1.296699
H	-2.892252	-3.846329	0.754736
H	-7.064210	2.001164	-3.298249
H	-8.556923	3.440306	-1.955484
H	-8.661464	3.175973	0.525124
H	-7.222259	1.499818	1.636924
H	-5.093951	0.570867	-3.361465
H	-4.573231	-0.386796	-1.987498
H	-5.201348	4.152280	0.087399
H	-5.313270	5.620664	1.111960
H	-3.735508	4.789750	0.910240
H	-4.051461	2.026262	4.799386
H	-4.826913	0.195023	6.271951
H	-5.860765	-1.852618	5.286954
H	-6.073774	-2.060178	2.834837
H	-3.119967	2.455614	2.352016
H	-4.221702	2.003548	1.053792

[$HPS_3BiCl_3Br]_2$ ('d' isomer) ωB97XD/def2-SVP (PCM)

E = -21725.253035

C	-7.235068	1.497196	0.319657
C	-6.340771	0.686392	-0.386423
C	-6.266157	0.730280	-1.798048
C	-7.077421	1.661158	-2.452596
C	-7.960899	2.480446	-1.749641
C	-8.054998	2.390274	-0.364508
P	-5.244263	-0.392399	0.546068
C	-5.208870	-0.031037	2.312007
C	-4.646810	1.170836	2.788243
C	-4.552796	1.342625	4.172925
C	-5.010599	0.369281	5.056425
C	-5.576634	-0.809205	4.573423
C	-5.670416	-1.012203	3.201424
C	-4.176068	2.275866	1.885113
S	-5.281938	3.725653	2.043830
C	-5.024701	4.485077	0.422750
C	-5.386139	-0.180459	-2.618394
S	-6.191459	-1.721805	-3.176216
C	-7.356727	-1.095042	-4.406922
C	-5.726478	-2.107759	0.288419
C	-4.779242	-3.148980	0.326560
C	-5.233776	-4.454989	0.129272
C	-6.586873	-4.724117	-0.073768
C	-7.516475	-3.688217	-0.084314
C	-7.083977	-2.377017	0.087646
C	-3.319024	-2.901095	0.577471
S	-2.413966	-2.252228	-0.871271
C	-2.485195	-3.659458	-1.997435
Bi	0.353648	-2.011398	0.562272
Br	-0.537764	-3.482887	2.724081

Br	1.054146	-4.296644	-0.846686
Br	2.758434	-1.507946	1.824367
Br	1.155885	-0.162357	-1.762911
Cl	-1.352601	0.200160	1.412905
Bi	-0.448612	2.240987	-0.537672
Br	-2.900791	2.042051	-1.760633
Cl	0.351052	3.844741	-2.407274
Br	-1.058282	4.310461	1.174898
S	2.501261	2.502235	0.526422
C	2.673661	4.057333	1.425642
C	3.337843	2.907711	-1.047008
C	4.808052	3.178556	-0.892286
C	5.758013	2.153312	-0.718992
C	7.120046	2.446128	-0.593821
C	7.556206	3.766377	-0.635645
C	6.625599	4.790809	-0.786230
C	5.268341	4.497668	-0.911770
P	5.277792	0.419125	-0.703773
C	6.355460	-0.508356	0.400359
C	6.263329	-0.330793	1.800937
C	7.057433	-1.152904	2.604769
C	7.939991	-2.081480	2.052987
C	8.049222	-2.213158	0.672375
C	7.248039	-1.430781	-0.154983
C	5.384633	0.703862	2.458201
S	6.196439	2.313939	2.749368
C	7.352514	1.895620	4.073075
C	5.265373	-0.220664	-2.390725
C	5.743116	0.603503	-3.419947
C	5.676089	0.178692	-4.742048
C	5.119887	-1.064672	-5.036924
C	4.645348	-1.882004	-4.015262
C	4.712938	-1.485800	-2.675695
C	4.216208	-2.424703	-1.613595
S	5.300918	-3.894650	-1.507738
C	4.959197	-4.388126	0.198178
H	3.968119	0.307077	-0.198312
H	2.210811	4.879564	0.863676
H	3.734138	4.261191	1.627596
H	2.140178	3.926320	2.375445
H	7.829280	2.836657	4.378847
H	8.133249	1.203438	3.727000
H	6.828602	1.464780	4.938491
H	4.547038	5.307804	-1.038696
H	6.956142	5.831018	-0.809620
H	8.619070	3.990847	-0.536453
H	7.845080	1.641447	-0.452916
H	3.128652	2.047962	-1.702661
H	2.820241	3.765469	-1.496225
H	6.974405	-1.067652	3.690247
H	8.544375	-2.708135	2.711667
H	8.736587	-2.938113	0.234278
H	7.303573	-1.562230	-1.236594

H	5.010344	0.320804	3.418747
H	4.492892	0.951035	1.864807
H	5.323079	-3.626251	0.903794
H	5.496513	-5.330065	0.372348
H	3.882715	-4.550206	0.347709
H	4.205810	-2.852896	-4.254929
H	5.049218	-1.400116	-6.073447
H	6.047454	0.824881	-5.538685
H	6.162080	1.585249	-3.192853
H	3.189106	-2.745814	-1.839340
H	4.184367	-1.965024	-0.615878
H	-3.936439	-0.199348	0.060394
H	-2.011371	-4.540550	-1.544312
H	-3.527358	-3.866191	-2.276856
H	-1.920038	-3.366254	-2.891405
H	-7.818786	-1.976066	-4.872475
H	-8.148058	-0.486899	-3.946531
H	-6.840777	-0.512707	-5.183948
H	-4.513612	-5.275770	0.149749
H	-6.914562	-5.755020	-0.220425
H	-8.576170	-3.894418	-0.240610
H	-7.808123	-1.560298	0.053332
H	-3.146669	-2.151629	1.366171
H	-2.821159	-3.819707	0.914844
H	-7.007306	1.752815	-3.538436
H	-8.578750	3.196738	-2.294604
H	-8.743171	3.028734	0.191056
H	-7.275875	1.452535	1.409011
H	-5.010614	0.357194	-3.500814
H	-4.495168	-0.521448	-2.072074
H	-5.404569	3.831426	-0.376546
H	-5.588057	5.427979	0.419476
H	-3.959311	4.694834	0.255659
H	-4.107300	2.261366	4.561308
H	-4.918451	0.530666	6.132139
H	-5.934979	-1.575651	5.262080
H	-6.095662	-1.943101	2.822015
H	-3.147093	2.564761	2.142617
H	-4.157928	1.986986	0.824617

[$HPS_3BiCl_3Br]_2$ ('e' isomer) ωB97XD/def2-SVP (PCM)

E = -21725.253440

C	-7.268494	1.430026	0.080603
C	-6.363590	0.511916	-0.461512
C	-6.262238	0.320632	-1.859454
C	-7.061464	1.125465	-2.675531
C	-7.956453	2.050043	-2.137252
C	-8.073648	2.195469	-0.758502
P	-5.279580	-0.392086	0.655309
C	-5.280371	0.254901	2.338953
C	-4.745857	1.528515	2.620890
C	-4.680011	1.926379	3.960035
C	-5.138919	1.102752	4.983804
C	-5.677954	-0.148773	4.691749

C	-5.742815	-0.575448	3.370179
C	-4.268305	2.475504	1.556602
S	-5.376579	3.928797	1.462390
C	-5.043799	4.444071	-0.238644
C	-5.363937	-0.708535	-2.499432
S	-6.156297	-2.327169	-2.798609
C	-7.257788	-1.931909	-4.175205
C	-5.736768	-2.133155	0.671856
C	-4.777032	-3.146448	0.862649
C	-5.219623	-4.471506	0.870974
C	-6.570563	-4.782617	0.721360
C	-7.511859	-3.770367	0.557822
C	-7.092470	-2.444327	0.523961
C	-3.315077	-2.856855	1.056898
S	-2.439141	-2.411264	-0.484029
C	-2.580891	-3.938078	-1.435024
Bi	0.431115	-2.120319	0.716663
Cl	-0.397290	-3.505859	2.737180
Br	1.103391	-4.392960	-0.713438
Br	2.864012	-1.648366	1.925839
Br	1.209437	-0.313200	-1.697306
Br	-1.209360	0.313222	1.697459
Bi	-0.431071	2.120217	-0.716696
Br	-2.863871	1.648073	-1.926044
Cl	0.397531	3.505520	-2.737250
Br	-1.103486	4.392987	0.713197
S	2.439042	2.411292	0.484154
C	2.580534	3.937895	1.435525
C	3.315118	2.857275	-1.056562
C	4.777075	3.146766	-0.862125
C	5.736769	2.133409	-0.671448
C	7.092469	2.444517	-0.523387
C	7.511903	3.770550	-0.556990
C	6.570651	4.782855	-0.720427
C	5.219713	4.471809	-0.870197
P	5.279567	0.392339	-0.655293
C	6.363465	-0.511938	0.461414
C	6.262076	-0.320895	1.859388
C	7.061031	-1.126100	2.675360
C	7.955844	-2.050777	2.136958
C	8.073128	-2.195930	0.758187
C	7.268214	-1.430128	-0.080823
C	5.364010	0.708411	2.499477
S	6.157004	2.326591	2.799453
C	7.257964	1.930232	4.176167
C	5.280424	-0.254313	-2.339074
C	5.742985	0.576210	-3.370109
C	5.678144	0.149821	-4.691773
C	5.138994	-1.101586	-4.984116
C	4.679966	-1.925386	-3.960541
C	4.745796	-1.527816	-2.621306
C	4.268101	-2.474997	-1.557250
S	5.376234	-3.928407	-1.463301

C	5.043480	-4.443865	0.237681
H	3.968855	0.267231	-0.156956
H	2.124020	4.776988	0.893883
H	3.635167	4.140079	1.668361
H	2.028676	3.769332	2.368877
H	7.708023	2.878734	4.498938
H	8.062790	1.247433	3.869258
H	6.700546	1.496378	5.018828
H	4.490169	5.272548	-1.008898
H	6.887298	5.827521	-0.735700
H	8.570021	4.008500	-0.440192
H	7.825674	1.649664	-0.370122
H	3.136974	2.004760	-1.730801
H	2.800573	3.713997	-1.511210
H	6.971509	-1.031712	3.759526
H	8.563165	-2.664757	2.804809
H	8.769949	-2.918450	0.331105
H	7.329732	-1.571402	-1.160881
H	4.978528	0.326054	3.455801
H	4.478703	0.943073	1.891559
H	5.401613	-3.686570	0.950972
H	5.589484	-5.382971	0.399750
H	3.968858	-4.616684	0.388322
H	4.254176	-2.902794	-4.198518
H	5.069570	-1.438511	-6.020237
H	6.037577	0.800919	-5.489871
H	6.147958	1.564249	-3.144624
H	3.243872	-2.809774	-1.776845
H	4.236430	-2.017200	-0.558568
H	-3.968916	-0.267065	0.156834
H	-2.124345	-4.777072	-0.893255
H	-3.635574	-4.140244	-1.667646
H	-2.029181	-3.769775	-2.368511
H	-7.707733	-2.880728	-4.497202
H	-8.062672	-1.249096	-3.868472
H	-6.700768	-1.498470	-5.018343
H	-4.490040	-5.272197	1.009755
H	-6.887177	-5.827290	0.736836
H	-8.569978	-4.008371	0.441143
H	-7.825710	-1.649524	0.370607
H	-3.136904	-2.004141	1.730877
H	-2.800418	-3.713413	1.511719
H	-6.972017	1.030856	-3.759685
H	-8.563976	2.663740	-2.805182
H	-8.770595	2.917927	-0.331519
H	-7.329954	1.571509	1.160637
H	-4.978844	-0.326322	-3.455971
H	-4.478385	-0.942635	-1.891653
H	-5.401992	3.686743	-0.951867
H	-5.589723	5.383207	-0.400801
H	-3.969166	4.616784	-0.389324
H	-4.254310	2.903881	4.197783
H	-5.069493	1.439911	6.019849

H	-6.037285	-0.799738	5.490002
H	-6.147696	-1.563575	3.144912
H	-3.244101	2.810437	1.776079
H	-4.236643	2.017478	0.558026

[$HPS_3BiCl_3Br]_2$ ('f' isomer) ωB97XD/def2-SVP (PCM)

E= -21725.257084

C	7.254142	1.409742	-0.129054
C	6.294793	0.613542	0.504892
C	6.139759	0.630163	1.910464
C	6.942102	1.517836	2.632423
C	7.892553	2.320465	2.001360
C	8.063369	2.257615	0.622145
P	5.229487	-0.416500	-0.515024
C	5.302706	0.014413	-2.264595
C	4.783452	1.241993	-2.724917
C	4.796789	1.479404	-4.103096
C	5.318104	0.545698	-4.994212
C	5.840170	-0.658718	-4.525717
C	5.827617	-0.926940	-3.161802
C	4.242823	2.302233	-1.807547
S	5.367655	3.747647	-1.765559
C	5.043736	4.342609	-0.088356
C	5.188219	-0.270318	2.657782
S	5.916963	-1.852772	3.205968
C	7.042450	-1.300917	4.506987
C	5.673769	-2.148558	-0.298389
C	4.717558	-3.176463	-0.411766
C	5.151187	-4.493871	-0.243479
C	6.491446	-4.786946	0.004870
C	7.430410	-3.763266	0.093007
C	7.018568	-2.442158	-0.050211
C	3.265476	-2.909786	-0.694032
S	2.341443	-2.284132	0.753291
C	2.466363	-3.674068	1.897018
Bi	-0.510390	-2.158262	-0.503795
Br	0.304004	-3.776440	-2.585501
Br	-1.138050	-4.322038	1.086424
Cl	-2.875250	-1.822073	-1.547541
Br	-1.141550	-0.173783	1.754443
Br	1.145633	0.173641	-1.753024
Bi	0.510840	2.158889	0.503024
Cl	2.875285	1.824070	1.547890
Br	-0.304345	3.778934	2.583263
Br	1.137242	4.322181	-1.088770
S	-2.341546	2.281793	-0.753755
C	-2.466729	3.671353	-1.897911
C	-3.265181	2.907786	0.693612
C	-4.717188	3.175306	0.411615
C	-5.673906	2.147872	0.298331
C	-7.018600	2.442085	0.050372
C	-7.429832	3.763415	-0.092668
C	-6.490384	4.786646	-0.004527
C	-5.150207	4.492931	0.243569

P	-5.230224	0.415755	0.515372
C	-6.296524	-0.614504	-0.503237
C	-6.142382	-0.631918	-1.908889
C	-6.945297	-1.519897	-2.629852
C	-7.895558	-2.321916	-1.997730
C	-8.065562	-2.258190	-0.618447
C	-7.255653	-1.410115	0.131782
C	-5.191275	0.268133	-2.657302
S	-5.920346	1.850362	-3.205758
C	-7.046735	1.297855	-4.505731
C	-5.302447	-0.014253	2.265199
C	-5.827914	0.927085	3.162114
C	-5.840067	0.659406	4.526130
C	-5.317038	-0.544442	4.995037
C	-4.795154	-1.478104	4.104224
C	-4.782236	-1.241258	2.725935
C	-4.241029	-2.301587	1.808997
S	-5.365988	-3.746933	1.766266
C	-5.043606	-4.340265	0.088174
H	-3.907623	0.218479	0.076330
H	-2.039324	4.579566	-1.452841
H	-3.514090	3.825718	-2.191285
H	-1.878117	3.392620	-2.781325
H	-7.465949	2.205882	-4.959786
H	-7.872195	0.695977	-4.099968
H	-6.512840	0.727579	-5.279609
H	-4.422283	5.303505	0.319684
H	-6.799563	5.826262	-0.127878
H	-8.479914	3.987525	-0.285201
H	-7.749696	1.636228	-0.043350
H	-3.115627	2.139845	1.469408
H	-2.765507	3.814388	1.060376
H	-6.816650	-1.590102	-3.711969
H	-8.506182	-3.003074	-2.593543
H	-8.806346	-2.883629	-0.118501
H	-7.358089	-1.387897	1.217777
H	-4.789396	-0.258680	-3.534430
H	-4.317165	0.559816	-2.058484
H	-5.382643	-3.605483	-0.656580
H	-5.612822	-5.271786	-0.033221
H	-3.973783	-4.544046	-0.055333
H	-4.382022	-2.416304	4.482016
H	-5.310193	-0.756472	6.065968
H	-6.247197	1.395652	5.220706
H	-6.222091	1.877014	2.796510
H	-3.246449	-2.624589	2.148507
H	-4.113644	-1.953318	0.774580
H	3.906374	-0.220149	-0.077115
H	2.038544	-4.581974	1.451706
H	3.513721	-3.828836	2.190160
H	1.877920	-3.395452	2.780583
H	7.461315	-2.209153	4.960953
H	7.868230	-0.698890	4.102091

H	6.508040	-0.730958	5.280749
H	4.423660	-5.304799	-0.319604
H	6.801090	-5.826402	0.128406
H	8.480569	-3.986882	0.285694
H	7.749284	-1.635967	0.043600
H	3.115486	-2.141977	-1.469847
H	2.766269	-3.816732	-1.060597
H	6.812807	1.587371	3.714508
H	8.502660	3.001413	2.597942
H	8.804254	2.883561	0.122985
H	7.357328	1.388149	-1.214986
H	4.785670	0.256087	3.534847
H	4.314573	-0.561819	2.058212
H	5.382695	3.608802	0.657382
H	5.612275	5.274613	0.032490
H	3.973684	4.545863	0.054195
H	4.384444	2.418081	-4.480563
H	5.311584	0.758168	-6.065058
H	6.246884	-1.394978	-5.220523
H	6.221083	-1.877293	-2.796528
H	3.247967	2.625276	-2.146248
H	4.116151	1.953826	-0.773078

[$HPS_3BiCl_3Br]_2$ ('g' isomer) ωB97XD/def2-SVP (PCM)

E= -21725.254648

C	-6.245099	0.796816	-1.729073
C	-6.326478	0.697261	-0.320389
C	-7.203403	1.501172	0.414337
C	-7.999459	2.440497	-0.235311
C	-7.902519	2.579822	-1.616035
C	-7.036561	1.767707	-2.348396
P	-5.247363	-0.433997	0.571345
C	-5.220921	-0.162599	2.355349
C	-4.682713	1.021605	2.899479
C	-4.593586	1.118759	4.291642
C	-5.031151	0.088899	5.119366
C	-5.572359	-1.072128	4.570698
C	-5.662046	-1.200517	3.189380
C	-4.222490	2.178941	2.058720
S	-5.294076	3.631296	2.348422
C	-4.850985	4.600870	0.887035
C	-5.371470	-0.088631	-2.583378
S	-6.186295	-1.598358	-3.208336
C	-7.341822	-0.912070	-4.416297
C	-5.735642	-2.131018	0.221844
C	-4.793792	-3.177061	0.180591
C	-5.259778	-4.465106	-0.094982
C	-6.616842	-4.713850	-0.296359
C	-7.540673	-3.675026	-0.226083
C	-7.097569	-2.380135	0.023365
C	-3.328504	-2.960390	0.434507
S	-2.422845	-2.234960	-0.977330
C	-2.506794	-3.576373	-2.181579
Bi	0.449545	-2.228629	0.250264

Cl	1.050194	-4.007085	-1.543698
Br	1.190278	0.006472	-1.723836
Bi	-0.449526	2.228633	-0.250261
Br	-1.190245	-0.006441	1.723876
Cl	-1.050163	4.007089	1.543698
Br	-2.898644	2.076001	-1.505757
Br	0.384119	4.152896	-2.052766
Br	2.898654	-2.076034	1.505786
Br	-0.384139	-4.152867	2.052759
S	2.422848	2.235009	0.977293
C	2.506823	3.576475	2.181483
C	3.328505	2.960366	-0.434583
C	4.793790	3.177061	-0.180680
C	5.735648	2.131024	-0.221899
C	7.097574	2.380156	-0.023434
C	7.540667	3.675058	0.225974
C	6.616829	4.713877	0.296217
C	5.259766	4.465118	0.094848
P	5.247372	0.433990	-0.571341
C	6.326488	-0.697247	0.320419
C	6.245090	-0.796785	1.729103
C	7.036549	-1.767665	2.348453
C	7.902515	-2.579788	1.616111
C	7.999470	-2.440481	0.235387
C	7.203421	-1.501166	-0.414286
C	5.371446	0.088670	2.583385
S	6.186242	1.598434	3.208293
C	7.341790	0.912213	4.416272
C	5.220906	0.162538	-2.355336
C	4.682705	-1.021694	-2.899413
C	4.593523	-1.118884	-4.291568
C	5.031033	-0.089038	-5.119338
C	5.572242	1.072015	-4.570725
C	5.661980	1.200447	-3.189415
C	4.222548	-2.179012	-2.058596
S	5.294082	-3.631384	-2.348393
C	4.850997	-4.601003	-0.887034
H	3.938087	0.223600	-0.098016
H	2.033572	4.481998	1.779358
H	3.550947	3.764246	2.466322
H	1.943240	3.237014	3.059617
H	7.809827	1.769589	4.918629
H	8.129297	0.316488	3.933509
H	6.818200	0.302811	5.166961
H	4.544816	5.289801	0.135827
H	6.952437	5.731765	0.503398
H	8.603612	3.865767	0.379785
H	7.816702	1.558667	-0.051909
H	3.142198	2.265817	-1.269075
H	2.838716	3.903993	-0.707407
H	6.961823	-1.898859	3.429937
H	8.502893	-3.330281	2.133988
H	8.672756	-3.073560	-0.344071

H	7.250293	-1.414442	-1.500776
H	4.987476	-0.482548	3.440941
H	4.485131	0.459441	2.049282
H	5.197177	-4.101497	0.029957
H	5.349632	-5.574805	-0.982541
H	3.763013	-4.748612	-0.840149
H	4.168102	-2.024697	-4.729338
H	4.943214	-0.193490	-6.202415
H	5.915848	1.882672	-5.214858
H	6.070250	2.117391	-2.761005
H	3.181937	-2.441752	-2.301075
H	4.245903	-1.959380	-0.981944
H	-3.938070	-0.223595	0.098043
H	-2.033501	-4.481896	-1.779503
H	-3.550916	-3.764169	-2.466409
H	-1.943239	-3.236852	-3.059707
H	-7.809911	-1.769420	-4.918651
H	-8.129292	-0.316308	-3.933519
H	-6.818211	-0.302693	-5.166991
H	-4.544835	-5.289795	-0.135983
H	-6.952458	-5.731729	-0.503571
H	-8.603619	-3.865719	-0.379904
H	-7.816692	-1.558643	0.051863
H	-3.142193	-2.265894	1.269042
H	-2.838733	-3.904044	0.707265
H	-6.961851	1.898911	-3.429881
H	-8.502903	3.330322	-2.133895
H	-8.672739	3.073569	0.344162
H	-7.250265	1.414431	1.500827
H	-4.987486	0.482603	-3.440917
H	-4.485164	-0.459437	-2.049283
H	-5.197157	4.101342	-0.029946
H	-5.349617	5.574677	0.982509
H	-3.762999	4.748471	0.840158
H	-4.168164	2.024552	4.729451
H	-4.943376	0.193319	6.202450
H	-5.916004	-1.882801	5.214789
H	-6.070324	-2.117438	2.760932
H	-3.181910	2.441690	2.301323
H	-4.245715	1.959321	0.982064

[$HPS_3BiCl_3Br]_2$ ('h' isomer) ωB97XD/def2-SVP (PCM)

E = -21725.256111

C	-4.590506	-1.195797	2.898530
C	-5.140502	0.015259	2.430684
C	-5.578322	1.000305	3.328074
C	-5.471203	0.793115	4.698425
C	-4.915770	-0.393898	5.172531
C	-4.482308	-1.371593	4.281694
P	-5.196679	0.385280	0.665873
C	-6.305431	-0.688333	-0.259026
C	-6.254505	-0.715946	-1.672277
C	-7.064887	-1.649723	-2.323427
C	-7.923512	-2.490289	-1.614790

C	-7.993022	-2.418592	-0.227234
C	-7.174806	-1.520719	0.452789
C	-5.395926	0.211332	-2.496604
S	-6.228209	1.745258	-3.035003
C	-7.384969	1.114216	-4.271477
C	-4.140993	-2.303227	1.987484
S	-5.229821	-3.758828	2.188427
C	-4.871460	-4.605128	0.630850
C	-5.674761	2.104236	0.423827
C	-4.725118	3.144412	0.444702
C	-5.184366	4.451874	0.267834
C	-6.541595	4.723914	0.099658
C	-7.472095	3.688960	0.103025
C	-7.036391	2.376556	0.256286
C	-3.256759	2.900004	0.652660
S	-2.397297	2.247731	-0.822309
C	-2.566479	3.622119	-1.979283
Bi	0.516888	2.134659	0.342207
Br	1.149489	4.187931	-1.386462
Br	-1.114483	-0.142783	1.707559
Cl	2.863650	1.848121	1.429249
Br	-0.238953	3.873005	2.351948
Br	1.221783	0.029858	-1.771603
Bi	-0.440581	-2.256548	-0.422056
Br	-2.907237	-2.021100	-1.637917
Br	0.438594	-4.049375	-2.330458
Cl	-1.060147	-4.155980	1.234565
S	2.373681	-2.301239	0.892306
C	2.414318	-3.683478	2.051509
C	3.344714	-2.964790	-0.506426
C	4.789947	-3.209322	-0.174864
C	5.738025	-2.171456	-0.093324
C	7.078414	-2.443451	0.199607
C	7.493109	-3.753045	0.419127
C	6.561353	-4.785816	0.362851
C	5.225633	-4.514035	0.070394
P	5.288784	-0.456694	-0.410904
C	5.423783	-0.114466	-2.177233
C	4.914911	1.083344	-2.719855
C	4.988452	1.253948	-4.106070
C	5.556972	0.284321	-4.926910
C	6.065251	-0.891591	-4.377868
C	5.993177	-1.093691	-3.004406
C	4.322143	2.181250	-1.882731
S	5.417239	3.649833	-1.879975
C	5.015836	4.328813	-0.252147
C	6.311334	0.633559	0.590597
C	7.279745	1.410146	-0.053640
C	8.057240	2.303979	0.677526
C	7.846977	2.430544	2.046742
C	6.887597	1.647443	2.688879
C	6.114648	0.717305	1.988670
C	5.148100	-0.152380	2.753342

S	5.860597	-1.711004	3.383745
C	6.990800	-1.102900	4.655481
H	-3.899372	0.192112	0.152868
H	-2.106194	4.531344	-1.570323
H	-3.626260	3.786339	-2.217858
H	-2.030134	3.325157	-2.889466
H	-7.863002	1.993013	-4.724949
H	-8.164670	0.486676	-3.817335
H	-6.860718	0.550813	-5.056884
H	-4.463495	5.272246	0.276013
H	-6.871413	5.756151	-0.032079
H	-8.534883	3.896586	-0.028271
H	-7.762091	1.560759	0.233814
H	-3.059129	2.153279	1.438273
H	-2.750670	3.820831	0.971295
H	-7.012417	-1.728255	-3.411312
H	-8.540674	-3.209046	-2.157318
H	-8.661510	-3.073528	0.333150
H	-7.198139	-1.489083	1.543031
H	-5.022504	-0.315780	-3.386272
H	-4.503602	0.560461	-1.957823
H	-5.242456	-4.019947	-0.223770
H	-5.391512	-5.571883	0.663507
H	-3.790792	-4.772721	0.524175
H	-4.046210	-2.297991	4.662322
H	-4.813447	-0.558939	6.246758
H	-5.811906	1.562612	5.392573
H	-5.996252	1.937412	2.956038
H	-3.103945	-2.591471	2.213331
H	-4.160226	-2.017979	0.925771
H	3.950171	-0.247490	-0.029800
H	1.985426	-4.583635	1.591923
H	3.442721	-3.859631	2.394769
H	1.789538	-3.385052	2.902851
H	7.402448	-1.990327	5.154849
H	7.821151	-0.528821	4.220498
H	6.460966	-0.490044	5.398921
H	4.504125	-5.332190	0.017823
H	6.873722	-5.815929	0.544208
H	8.540057	-3.960759	0.644481
H	7.803024	-1.629134	0.267504
H	3.210934	-2.224109	-1.310753
H	2.862570	-3.887304	-0.856005
H	6.727832	1.766162	3.762567
H	8.432804	3.146351	2.626613
H	8.805251	2.913997	0.169347
H	7.415613	1.335558	-1.133544
H	4.728234	0.411729	3.598360
H	4.287412	-0.469794	2.148303
H	5.337390	3.642710	0.544856
H	5.562837	5.276846	-0.160025
H	3.937312	4.517878	-0.162402
H	4.586349	2.169550	-4.545958

H	5.599505	0.446678	-6.005631
H	6.508469	-1.656617	-5.016956
H	6.376773	-2.021708	-2.576805
H	3.333648	2.463259	-2.273067
H	4.165235	1.888751	-0.835659

$[HPS_3BiCl_3Br]_2$ ('i' isomer) ωB97XD/def2-SVP (PCM)

E=-21725.255225

C	-4.678630	-1.453282	2.656812
C	-5.205871	-0.191095	2.315364
C	-5.671059	0.686175	3.305618
C	-5.616254	0.318303	4.645090
C	-5.084756	-0.921384	4.995937
C	-4.623138	-1.791737	4.012735
P	-5.187134	0.383216	0.606092
C	-6.269007	-0.556903	-0.482316
C	-6.163733	-0.410317	-1.885120
C	-6.961787	-1.239399	-2.677770
C	-7.859493	-2.145104	-2.112959
C	-7.980302	-2.246672	-0.730497
C	-7.176644	-1.456034	0.086415
C	-5.260961	0.596087	-2.554434
S	-6.058090	2.194685	-2.936641
C	-7.114985	1.740428	-4.330131
C	-4.196102	-2.447587	1.638629
S	-5.309214	-3.900280	1.601109
C	-4.983456	-4.486370	-0.078020
C	-5.632878	2.126603	0.544044
C	-4.670121	3.144095	0.695085
C	-5.108350	4.469645	0.643445
C	-6.457378	4.779093	0.474251
C	-7.401445	3.764231	0.349179
C	-6.986425	2.436572	0.374535
C	-3.208572	2.861341	0.906372
S	-2.330364	2.334961	-0.607194
C	-2.476972	3.805364	-1.642269
Bi	0.565578	2.068918	0.561035
Br	1.171224	4.285750	-0.967643
Br	-1.114273	-0.307101	1.666075
Cl	2.940074	1.692402	1.561470
Br	-0.179765	3.603219	2.729607
Br	1.240458	0.190363	-1.783041
Bi	-0.397906	-2.210510	-0.681976
Br	-2.832917	-1.808745	-1.917817
Cl	0.488115	-3.677372	-2.619621
Br	-1.066928	-4.422664	0.833107
S	2.425791	-2.370737	0.608899
C	2.540754	-3.809545	1.691488
C	3.355941	-2.934428	-0.859725
C	4.809301	-3.200708	-0.584935
C	5.758216	-2.171097	-0.431060
C	7.104568	-2.464981	-0.191442
C	7.525382	-3.787723	-0.098247
C	6.593822	-4.813727	-0.227530

C	5.251920	-4.520516	-0.466830
P	5.303378	-0.434542	-0.580558
C	5.383351	0.067428	-2.311113
C	4.859420	1.309507	-2.725268
C	4.870553	1.597663	-4.093834
C	5.392669	0.698463	-5.019426
C	5.918848	-0.520850	-4.596363
C	5.909334	-0.838885	-3.243060
C	4.314717	2.332083	-1.768121
S	5.429575	3.782683	-1.678880
C	5.069899	4.337984	0.004744
C	6.352291	0.556734	0.494117
C	7.300197	1.402079	-0.091371
C	8.092645	2.221399	0.707971
C	7.918426	2.204297	2.088141
C	6.979896	1.352407	2.670357
C	6.192684	0.494424	1.897950
C	5.247765	-0.455378	2.590777
S	5.994104	-2.051322	3.071764
C	7.063228	-1.551180	4.439699
H	-3.872496	0.230722	0.126344
H	-2.019778	4.674019	-1.149949
H	-3.532354	3.992792	-1.883883
H	-1.926378	3.585134	-2.565661
H	-7.551857	2.674675	-4.708061
H	-7.931080	1.072319	-4.020765
H	-6.531119	1.270282	-5.134673
H	-4.376760	5.273415	0.750304
H	-6.769734	5.824644	0.442200
H	-8.458035	4.000395	0.216218
H	-7.721890	1.638736	0.250145
H	-3.032785	2.045799	1.625570
H	-2.698298	3.744002	1.314240
H	-6.868792	-1.179610	-3.764084
H	-8.466304	-2.778580	-2.762836
H	-8.679022	-2.954636	-0.282630
H	-7.241056	-1.564282	1.170114
H	-4.857561	0.175865	-3.487030
H	-4.386322	0.861940	-1.943790
H	-5.337563	-3.755782	-0.820417
H	-5.536913	-5.427142	-0.200475
H	-3.910434	-4.672833	-0.223277
H	-4.203181	-2.759265	4.297053
H	-5.022814	-1.211618	6.046548
H	-5.977137	1.005687	5.411474
H	-6.069293	1.665150	3.033207
H	-3.174894	-2.775729	1.881072
H	-4.154059	-2.034267	0.620754
H	3.975131	-0.263826	-0.146998
H	2.110908	-4.695954	1.206514
H	3.586628	-3.980499	1.981202
H	1.950650	-3.566274	2.584302
H	7.482629	-2.474894	4.860846

H	7.891620	-0.915073	4.096883
H	6.491628	-1.031319	5.222197
H	4.529660	-5.332453	-0.575289
H	6.910718	-5.854958	-0.143248
H	8.576704	-4.011260	0.088047
H	7.829694	-1.658176	-0.065285
H	3.200888	-2.139564	-1.606333
H	2.860737	-3.828227	-1.261296
H	6.846708	1.359172	3.754159
H	8.516303	2.861089	2.722983
H	8.823808	2.886674	0.246713
H	7.407858	1.442028	-1.176263
H	4.828472	0.022522	3.487664
H	4.384187	-0.729752	1.969258
H	5.400000	3.589940	0.740303
H	5.628711	5.271125	0.157701
H	3.995706	4.530346	0.131008
H	4.454883	2.548340	-4.435876
H	5.383265	0.949809	-6.081841
H	6.326045	-1.230521	-5.318055
H	6.305865	-1.800926	-2.913489
H	3.315512	2.659782	-2.089514
H	4.196526	1.943901	-0.746829

[$HPS_3BiCl_3Br]_2$ ('j' isomer) ωB97XD/def2-SVP (PCM)

E= -21725.254058

C	-4.762012	1.249069	-2.680543
C	-5.284844	0.014394	-2.243874
C	-5.776641	-0.924209	-3.162476
C	-5.751215	-0.646465	-4.524342
C	-5.223770	0.564595	-4.968992
C	-4.736439	1.496269	-4.056711
P	-5.239453	-0.440682	-0.499448
C	-6.303488	0.579188	0.532503
C	-6.176113	0.543493	1.940736
C	-6.966662	1.429625	2.677435
C	-7.878566	2.283353	2.056857
C	-8.021884	2.274137	0.673057
C	-7.225266	1.426118	-0.091363
C	-5.260811	-0.404213	2.675844
S	-6.036234	-1.980348	3.175665
C	-7.155451	-1.432928	4.484059
C	-4.255471	2.306257	-1.740218
S	-5.358870	3.766136	-1.776501
C	-5.019263	4.442945	-0.134534
C	-5.694438	-2.172566	-0.307394
C	-4.739349	-3.203197	-0.403990
C	-5.180567	-4.519665	-0.247979
C	-6.526843	-4.809038	-0.029515
C	-7.464380	-3.782656	0.039782
C	-7.045301	-2.462443	-0.089252
C	-3.283428	-2.941540	-0.669150
S	-2.360059	-2.346110	0.790989
C	-2.412067	-3.793207	1.867901

Bi	0.480454	-2.169356	-0.473243
Cl	1.112620	-4.151054	1.085499
Br	-1.210360	0.149950	-1.689013
Br	2.945344	-1.850945	-1.673185
Br	-0.344806	-3.868249	-2.486364
Br	1.187161	-0.155608	1.753023
Bi	-0.404241	2.196413	0.506333
Br	-2.821238	1.879944	1.788985
Cl	0.438518	3.764077	2.385244
Br	-1.075032	4.322939	-1.126305
S	2.488304	2.334118	-0.677553
C	2.645660	3.765656	-1.764942
C	3.348514	2.917537	0.825670
C	4.817673	3.163292	0.627813
C	5.763304	2.120940	0.563138
C	7.125382	2.395261	0.402458
C	7.565945	3.711209	0.302208
C	6.639583	4.748948	0.343923
C	5.281732	4.475079	0.503780
P	5.279072	0.394401	0.731875
C	5.234938	-0.058348	2.477587
C	4.670390	-1.282120	2.892776
C	4.575734	-1.523434	4.267036
C	5.036254	-0.597380	5.198668
C	5.606516	0.601963	4.775920
C	5.700798	0.874101	3.415941
C	4.191434	-2.335008	1.933299
S	5.268116	-3.811120	2.031517
C	4.919776	-4.536151	0.412021
C	6.376035	-0.641807	-0.248324
C	7.241693	-1.515199	0.417654
C	8.050080	-2.384719	-0.309446
C	7.973873	-2.388209	-1.698498
C	7.118911	-1.507281	-2.360835
C	6.319590	-0.599601	-1.661011
C	5.468287	0.375550	-2.436233
S	6.317695	1.922385	-2.906795
C	7.453863	1.337444	-4.184142
H	-3.917082	-0.259474	-0.050513
H	-1.941032	-4.655334	1.377676
H	-3.449411	-4.013441	2.154486
H	-1.833797	-3.529482	2.762449
H	-7.597741	-2.341796	4.913970
H	-7.964904	-0.802056	4.090337
H	-6.612413	-0.894632	5.274457
H	-4.454050	-5.332502	-0.312686
H	-6.842582	-5.847793	0.084236
H	-8.519153	-4.003396	0.208954
H	-7.775372	-1.654425	-0.006775
H	-3.122440	-2.164913	-1.433762
H	-2.788210	-3.846765	-1.044268
H	-6.856992	1.457832	3.763524
H	-8.479676	2.962172	2.664840

H	-8.732075	2.940309	0.181388
H	-7.308193	1.445634	-1.179019
H	-4.856003	0.087069	3.572322
H	-4.387652	-0.707367	2.080617
H	-5.371217	3.755377	0.648883
H	-5.569065	5.390876	-0.060162
H	-3.944800	4.633037	-0.005693
H	-4.320480	2.440622	-4.415411
H	-5.185635	0.784046	-6.037751
H	-6.132205	-1.380687	-5.235636
H	-6.172918	-1.880178	-2.815402
H	-3.236285	2.610336	-2.020596
H	-4.199267	1.960026	-0.698555
H	3.977807	0.229749	0.218538
H	2.186646	4.652215	-1.307489
H	3.703311	3.944076	-2.002924
H	2.103175	3.513586	-2.684976
H	7.937714	2.231141	-4.600819
H	8.230625	0.679752	-3.769220
H	6.915038	0.817997	-4.989880
H	4.563454	5.296599	0.546206
H	6.973142	5.784444	0.253364
H	8.629184	3.919758	0.176217
H	7.848350	1.578782	0.343429
H	3.146011	2.139766	1.578737
H	2.841617	3.823080	1.183602
H	7.060902	-1.531907	-3.450943
H	8.583227	-3.083929	-2.278554
H	8.716412	-3.071007	0.214834
H	7.270763	-1.538117	1.507932
H	5.084677	-0.104620	-3.347903
H	4.582140	0.709955	-1.878165
H	5.285366	-3.880646	-0.392439
H	5.451209	-5.496362	0.369180
H	3.841282	-4.707098	0.290612
H	4.127866	-2.459654	4.607901
H	4.943206	-0.812085	6.264978
H	5.967770	1.331685	5.501942
H	6.130007	1.821581	3.085414
H	3.155392	-2.624539	2.161551
H	4.194279	-1.992443	0.888511

[$HPS_3BiCl_3I]_2$ ('a' isomer) ωB97XD/def2-SVP (PCM)

E= -8068.486605

C	4.673224	-0.565027	-2.904917
C	5.246539	0.565241	-2.288182
C	5.619948	1.686766	-3.042745
C	5.427852	1.694313	-4.419481
C	4.852140	0.586607	-5.039393
C	4.480973	-0.525746	-4.289381
P	5.390386	0.655852	-0.494144
C	6.540598	-0.535722	0.207397
C	6.550758	-0.774154	1.601655
C	7.396811	-1.782164	2.072231

C	8.229714	-2.496565	1.211191
C	8.235959	-2.220645	-0.152826
C	7.382897	-1.242679	-0.656563
C	5.720237	0.008408	2.590039
S	6.564141	1.448291	3.331043
C	7.736606	0.643910	4.445806
C	4.279325	-1.800879	-2.146429
S	5.341076	-3.208923	-2.630244
C	5.182289	-4.228997	-1.146120
C	5.862179	2.318504	0.004974
C	4.894572	3.325252	0.189290
C	5.334877	4.588795	0.589538
C	6.691816	4.855787	0.769256
C	7.640175	3.860589	0.551894
C	7.223574	2.586154	0.179961
C	3.429905	3.095093	-0.059453
S	2.561919	2.147347	1.237575
C	2.693766	3.274135	2.639793
Bi	-0.316178	2.119541	-0.275151
I	-1.008109	4.394113	1.568575
Cl	1.275958	0.001136	-1.399385
Bi	0.328238	-2.241995	0.221276
I	2.925912	-2.139086	1.622161
I	-0.458248	-4.493279	2.057581
I	1.012486	-4.089432	-2.004479
Cl	-1.229522	-0.038627	1.477158
I	-2.847532	1.873623	-1.768975
I	0.711926	3.949165	-2.424613
S	-2.710609	-2.333041	-0.850490
C	-2.970210	-3.743341	-1.946500
C	-3.539188	-2.913473	0.671724
C	-5.010936	-3.169310	0.506813
C	-5.966117	-2.135399	0.494310
C	-7.330183	-2.411506	0.358912
C	-7.762705	-3.727610	0.228996
C	-6.827647	-4.759000	0.219807
C	-5.468069	-4.480876	0.356447
P	-5.468132	-0.425615	0.729361
C	-5.338708	-0.075012	2.492724
C	-4.712938	1.104640	2.942100
C	-4.556642	1.277267	4.320944
C	-5.018313	0.324687	5.224818
C	-5.647870	-0.832510	4.768829
C	-5.802570	-1.036323	3.402500
C	-4.236746	2.183811	2.012514
S	-5.274627	3.678791	2.200966
C	-5.100006	4.389076	0.547248
C	-6.591704	0.678444	-0.138394
C	-7.423051	1.511338	0.617467
C	-8.253231	2.429619	-0.019086
C	-8.230552	2.523735	-1.407146
C	-7.409877	1.683297	-2.159611
C	-6.592929	0.725873	-1.552151

C	-5.789370	-0.212794	-2.418050
S	-6.685269	-1.717114	-2.938646
C	-7.854605	-1.045882	-4.141710
H	4.117346	0.372857	0.037060
H	2.221835	4.238645	2.408562
H	3.748045	3.407823	2.919331
H	2.156629	2.798904	3.470634
H	8.216753	1.447287	5.020763
H	8.514104	0.096088	3.894775
H	7.222393	-0.033537	5.142713
H	4.599844	5.381587	0.745069
H	7.007667	5.854797	1.075933
H	8.702660	4.066619	0.687962
H	7.962954	1.794743	0.039299
H	3.253658	2.524970	-0.985103
H	2.913658	4.055220	-0.190942
H	7.395238	-2.018674	3.138357
H	8.876674	-3.278397	1.613570
H	8.882845	-2.778788	-0.830927
H	7.355362	-1.051131	-1.730404
H	5.387155	-0.652681	3.403555
H	4.804982	0.426138	2.145241
H	5.631599	-3.725095	-0.277117
H	5.724110	-5.164140	-1.341612
H	4.127673	-4.459095	-0.939638
H	4.025069	-1.387128	-4.782805
H	4.684661	0.590372	-6.118128
H	5.717355	2.569451	-5.003019
H	6.052678	2.561946	-2.554650
H	3.224841	-2.042441	-2.344372
H	4.369708	-1.679475	-1.058160
H	-4.187438	-0.247256	0.170230
H	-2.550625	-4.658478	-1.506681
H	-4.040521	-3.867980	-2.160877
H	-2.436320	-3.514475	-2.877698
H	-8.371971	-1.908807	-4.582337
H	-8.601665	-0.395145	-3.665864
H	-7.334485	-0.498692	-4.941220
H	-4.743747	-5.298245	0.359268
H	-7.156433	-5.793903	0.107761
H	-8.826882	-3.941685	0.121450
H	-8.058050	-1.597449	0.345312
H	-3.315912	-2.136777	1.420174
H	-3.031610	-3.824211	1.014451
H	-7.396857	1.777654	-3.247424
H	-8.855719	3.260227	-1.915572
H	-8.893559	3.083829	0.574032
H	-7.404580	1.463864	1.707360
H	-5.437642	0.311540	-3.318579
H	-4.888579	-0.595170	-1.916197
H	-5.539856	3.723195	-0.210432
H	-5.647221	5.341418	0.551929
H	-4.043823	4.579123	0.310721

H	-4.061103	2.179197	4.687381
H	-4.879800	0.485443	6.295615
H	-6.008718	-1.582332	5.474252
H	-6.277144	-1.951443	3.044057
H	-3.186696	2.430319	2.226014
H	-4.277326	1.886355	0.955412

[$HPS_3BiCl_3I]_2$ ('b' isomer) ωB97XD/def2-SVP (PCM)

E= -8068.494324

C	7.353504	1.481101	-0.143444
C	6.374930	0.803503	0.590529
C	6.117459	1.122942	1.943909
C	6.842080	2.180013	2.500414
C	7.810938	2.865306	1.767814
C	8.079830	2.510270	0.449475
P	5.417087	-0.481310	-0.225272
C	5.591768	-0.500210	-2.019790
C	5.068818	0.547283	-2.806056
C	5.142140	0.415896	-4.196670
C	5.721804	-0.701590	-4.790567
C	6.244960	-1.725002	-4.002515
C	6.174558	-1.627090	-2.617725
C	4.471792	1.799304	-2.225659
S	5.589097	3.219902	-2.525996
C	5.181177	4.256473	-1.100667
C	5.125633	0.379676	2.804828
S	5.832924	-0.995060	3.776285
C	6.759034	-0.100388	5.044098
C	5.889724	-2.084228	0.449717
C	4.975767	-3.152801	0.531056
C	5.425456	-4.360623	1.069107
C	6.746436	-4.516832	1.487117
C	7.648052	-3.462540	1.375340
C	7.215771	-2.242310	0.865485
C	3.554282	-3.037847	0.057174
S	2.467846	-2.093825	1.181029
C	2.440988	-3.150148	2.642233
Bi	-0.163773	-2.172262	-0.480951
I	1.015764	-3.819338	-2.669569
I	-0.980899	-4.590929	1.096341
I	-2.667811	-1.640693	-1.987715
I	-0.915576	-0.102424	1.993294
Cl	1.455890	0.014412	-1.468529
Bi	0.627617	2.292059	0.130140
Cl	3.023281	2.230068	1.079030
I	0.019170	4.541251	2.015665
I	1.123511	4.074291	-2.175134
S	-2.511363	2.455099	-0.655509
C	-2.799819	3.922281	-1.667499
C	-3.278070	2.966047	0.922707
C	-4.751535	3.253191	0.829081
C	-5.728404	2.241078	0.750877
C	-7.090632	2.555216	0.696272
C	-7.500822	3.884187	0.712483

C	-6.545331	4.895201	0.765252
C	-5.188251	4.580556	0.821617
P	-5.282144	0.498633	0.757305
C	-6.435573	-0.440837	-0.256108
C	-6.416323	-0.311249	-1.664765
C	-7.264478	-1.146149	-2.397138
C	-8.130998	-2.039422	-1.767063
C	-8.169601	-2.121519	-0.378878
C	-7.312912	-1.326668	0.377879
C	-5.562386	0.690560	-2.401210
S	-6.374412	2.300943	-2.693210
C	-7.588794	1.862843	-3.956640
C	-5.167408	-0.104084	2.452904
C	-5.530742	0.763134	3.493196
C	-5.369363	0.369631	4.816806
C	-4.834088	-0.885521	5.100504
C	-4.473520	-1.746058	4.067567
C	-4.636105	-1.380423	2.727801
C	-4.247599	-2.355975	1.653612
S	-5.352974	-3.811751	1.680108
C	-5.131288	-4.377289	-0.022425
H	-4.009763	0.360992	0.170477
H	-2.359025	4.809570	-1.192792
H	-3.876107	4.061371	-1.838938
H	-2.298513	3.741278	-2.626836
H	-8.072842	2.800873	-4.260120
H	-8.357778	1.183089	-3.563018
H	-7.104698	1.411917	-4.834802
H	-4.447661	5.381518	0.873629
H	-6.855329	5.941952	0.765522
H	-8.563802	4.125358	0.668930
H	-7.836255	1.760003	0.628136
H	-3.050623	2.147420	1.623298
H	-2.739189	3.848533	1.293191
H	-7.239330	-1.099038	-3.487909
H	-8.778368	-2.677642	-2.371474
H	-8.844232	-2.818455	0.120066
H	-7.311873	-1.420802	1.464948
H	-5.248956	0.277141	-3.371000
H	-4.636261	0.945104	-1.865498
H	-5.527611	-3.636264	-0.733153
H	-5.694672	-5.314421	-0.125044
H	-4.070219	-4.568550	-0.235997
H	-4.047429	-2.725170	4.297908
H	-4.690021	-1.195965	6.137128
H	-5.652060	1.048671	5.622395
H	-5.933142	1.753278	3.271977
H	-3.208847	-2.685930	1.802563
H	-4.297120	-1.921772	0.645208
H	4.058858	-0.237831	0.053045
H	2.084199	-4.157745	2.389156
H	3.438945	-3.184171	3.100786
H	1.735706	-2.682541	3.341664

H	7.125467	-0.855636	5.752556
H	7.623307	0.429363	4.619369
H	6.112897	0.607293	5.583334
H	4.728544	-5.197937	1.147164
H	7.071687	-5.473646	1.899871
H	8.683515	-3.581250	1.697313
H	7.914960	-1.405774	0.803845
H	3.476969	-2.511594	-0.907230
H	3.117469	-4.033752	-0.098131
H	6.634905	2.478991	3.529941
H	8.355357	3.688679	2.234227
H	8.834588	3.045114	-0.128721
H	7.532524	1.227016	-1.189356
H	4.633337	1.079837	3.494625
H	4.315916	-0.080352	2.221899
H	5.472723	3.763552	-0.162147
H	5.752130	5.187773	-1.215780
H	4.108019	4.489531	-1.075768
H	4.731291	1.210861	-4.823330
H	5.760826	-0.776377	-5.879004
H	6.697759	-2.604584	-4.462204
H	6.566439	-2.437929	-2.001202
H	3.490204	1.993348	-2.681907
H	4.298557	1.734026	-1.142833

[$HPS_3BiCl_3I]_2$ ('c' isomer) ωB97XD/def2-SVP (PCM)

E = -8068.490693

C	-7.266970	1.418691	1.122034
C	-6.514148	0.781551	0.130488
C	-6.582408	1.192945	-1.221321
C	-7.383144	2.300644	-1.513209
C	-8.122187	2.947665	-0.523011
C	-8.079229	2.500291	0.793805
P	-5.378086	-0.525102	0.619922
C	-5.160277	-0.692282	2.403068
C	-4.532472	0.320554	3.157285
C	-4.279387	0.064381	4.508615
C	-4.642167	-1.142868	5.098285
C	-5.273919	-2.131340	4.346101
C	-5.528093	-1.908264	2.998058
C	-4.149278	1.658211	2.588401
S	-5.156613	2.974917	3.360201
C	-4.883224	4.289029	2.148536
C	-5.857036	0.494273	-2.346406
S	-6.847701	-0.762275	-3.228126
C	-7.944363	0.278248	-4.218542
C	-5.917032	-2.094107	-0.079399
C	-4.991576	-3.112017	-0.385504
C	-5.482948	-4.305281	-0.918108
C	-6.850636	-4.497349	-1.114801
C	-7.756756	-3.495820	-0.780687
C	-7.288060	-2.287764	-0.272127
C	-3.519365	-2.965868	-0.123407
S	-2.610911	-1.959051	-1.346430

C	-2.706765	-3.009519	-2.810085
Bi	0.206249	-2.120559	0.153165
I	-0.847310	-4.039566	2.205502
I	1.025007	-4.298007	-1.733753
I	2.703598	-1.829886	1.709616
I	1.058536	0.226512	-2.001407
Cl	-1.381187	-0.032632	1.374143
Bi	-0.494667	2.424214	0.056975
I	-3.143412	2.618692	-1.205653
I	0.321718	4.915671	-1.406619
Cl	-1.016985	3.702031	2.242198
S	2.564209	2.399181	1.062279
C	2.680180	3.766604	2.236307
C	3.448566	3.091361	-0.378666
C	4.911161	3.344984	-0.140683
C	5.877159	2.320568	-0.170306
C	7.234303	2.601004	0.018557
C	7.648646	3.909183	0.247350
C	6.701837	4.928261	0.304691
C	5.349726	4.647260	0.112280
P	5.413839	0.612931	-0.488546
C	6.512575	-0.502113	0.398498
C	6.436577	-0.607406	1.807322
C	7.238632	-1.573354	2.420961
C	8.114520	-2.369945	1.683085
C	8.211468	-2.219287	0.303468
C	7.401106	-1.288898	-0.341245
C	5.569124	0.278440	2.667093
S	6.391855	1.793488	3.269534
C	7.566109	1.115942	4.464272
C	5.356948	0.307022	-2.264755
C	5.775115	1.331259	-3.126721
C	5.660358	1.173706	-4.503189
C	5.117192	-0.002151	-5.017721
C	4.702219	-1.018380	-4.161790
C	4.817297	-0.891818	-2.774111
C	4.377820	-2.032821	-1.900591
S	5.472833	-3.477107	-2.139651
C	5.190796	-4.317216	-0.563542
H	4.116923	0.399530	0.017957
H	2.269836	4.684853	1.794211
H	3.721998	3.913624	2.551670
H	2.067552	3.482231	3.101128
H	8.044068	1.977439	4.949909
H	8.344154	0.514099	3.973834
H	7.054207	0.515475	5.229997
H	4.616930	5.456537	0.143408
H	7.015394	5.956331	0.495405
H	8.707503	4.125759	0.395008
H	7.970849	1.794874	-0.000633
H	3.269896	2.369228	-1.191179
H	2.941445	4.019220	-0.674645
H	7.168097	-1.710017	3.502034

H	8.724299	-3.116130	2.196042
H	8.893733	-2.839528	-0.279274
H	7.444605	-1.196054	-1.427484
H	5.199119	-0.286061	3.535543
H	4.677241	0.649737	2.141815
H	5.581244	-3.716643	0.271941
H	5.733055	-5.271256	-0.606841
H	4.120511	-4.516237	-0.411887
H	4.271575	-1.933840	-4.573793
H	5.009047	-0.128326	-6.096583
H	5.985466	1.973164	-5.170434
H	6.183653	2.259228	-2.722498
H	3.341643	-2.316381	-2.139501
H	4.392125	-1.780430	-0.831029
H	-4.114115	-0.203595	0.086689
H	-2.240274	-3.985622	-2.618868
H	-3.753032	-3.128422	-3.123553
H	-2.148262	-2.490296	-3.599621
H	-8.515887	-0.401638	-4.864745
H	-8.651340	0.839523	-3.591810
H	-7.370788	0.971001	-4.851028
H	-4.780943	-5.104564	-1.165001
H	-7.208224	-5.442535	-1.527686
H	-8.827108	-3.643784	-0.929577
H	-7.994985	-1.490088	-0.035427
H	-3.319678	-2.473495	0.841394
H	-3.042915	-3.953644	-0.064183
H	-7.417684	2.674753	-2.538447
H	-8.733229	3.812974	-0.787327
H	-8.653901	3.002611	1.573191
H	-7.198638	1.093381	2.161103
H	-5.506839	1.231614	-3.083221
H	-4.959385	-0.044728	-2.009906
H	-5.366934	4.042579	1.191548
H	-5.333069	5.203559	2.557722
H	-3.807155	4.448873	1.992581
H	-3.783469	0.833236	5.105353
H	-4.426665	-1.314446	6.154569
H	-5.559426	-3.079866	4.802959
H	-6.005872	-2.690397	2.405262
H	-3.083850	1.861656	2.769057
H	-4.299056	1.715606	1.500666

[$HPS_3BiCl_3I]_2$ ('d' isomer) ωB97XD/def2-SVP (PCM)

E= -8068.491180

C	-7.353389	1.193426	0.590451
C	-6.478568	0.585997	-0.315926
C	-6.490443	0.925068	-1.689165
C	-7.367360	1.936910	-2.089945
C	-8.232880	2.552574	-1.185768
C	-8.240294	2.172993	0.152848
P	-5.295487	-0.613885	0.310895
C	-5.092251	-0.596576	2.101957
C	-4.546869	0.527763	2.754894

C	-4.262804	0.414963	4.119104
C	-4.516817	-0.762494	4.816536
C	-5.071232	-1.861744	4.163757
C	-5.355206	-1.780558	2.805555
C	-4.280264	1.834586	2.061599
S	-5.437834	3.111640	2.669984
C	-5.316933	4.287907	1.302421
C	-5.636151	0.244176	-2.730902
S	-6.427870	-1.174908	-3.565420
C	-7.727005	-0.358165	-4.518569
C	-5.759292	-2.261881	-0.250455
C	-4.796613	-3.277824	-0.417327
C	-5.230487	-4.523308	-0.874785
C	-6.580324	-4.767671	-1.127832
C	-7.525952	-3.767391	-0.925085
C	-7.113058	-2.509313	-0.496347
C	-3.348635	-3.073583	-0.072639
S	-2.386885	-2.088484	-1.269984
C	-2.282528	-3.227994	-2.663795
Bi	0.233809	-1.965550	0.520710
I	-1.015190	-3.315491	2.886372
I	1.042584	-4.576259	-0.762747
I	2.716086	-1.333541	2.012063
I	1.083501	-0.112383	-2.088927
Cl	-1.356559	0.267678	1.236397
Bi	-0.374152	2.511497	-0.399740
I	-3.000587	2.581296	-1.722169
Cl	0.438314	4.492932	-1.878478
I	-1.004574	4.277010	1.883476
S	2.732796	2.643660	0.395313
C	2.952151	4.271879	1.145732
C	3.456981	2.937080	-1.258608
C	4.933037	3.219230	-1.221856
C	5.897323	2.208264	-1.041500
C	7.263202	2.508258	-1.017756
C	7.690055	3.823093	-1.171891
C	6.747383	4.834757	-1.334879
C	5.386125	4.533998	-1.357738
P	5.425408	0.479885	-0.882950
C	6.564858	-0.383257	0.210834
C	6.542355	-0.136850	1.604042
C	7.379899	-0.916649	2.406143
C	8.238230	-1.869092	1.856549
C	8.279852	-2.067271	0.480207
C	7.434263	-1.328714	-0.343117
C	5.696850	0.929608	2.253713
S	6.508940	2.559655	2.394922
C	7.782732	2.225188	3.631686
C	5.296685	-0.274144	-2.515689
C	5.680158	0.483320	-3.631895
C	5.516552	-0.032447	-4.912560
C	4.958076	-1.298649	-5.078429
C	4.575725	-2.049095	-3.970197

C	4.741154	-1.560266	-2.670858
C	4.334131	-2.423956	-1.510961
S	5.418122	-3.891870	-1.399817
C	5.184082	-4.290934	0.347769
H	4.153311	0.412070	-0.284549
H	2.448565	5.033005	0.533663
H	4.020915	4.497570	1.261649
H	2.478697	4.226586	2.134713
H	8.275958	3.185512	3.833799
H	8.535273	1.515772	3.258910
H	7.343054	1.847099	4.565881
H	4.655187	5.334022	-1.493867
H	7.071429	5.871017	-1.448239
H	8.755970	4.054400	-1.152562
H	7.998288	1.714723	-0.866670
H	3.211590	2.035120	-1.840613
H	2.903711	3.765739	-1.721089
H	7.353053	-0.777016	3.488947
H	8.876894	-2.462089	2.513959
H	8.949054	-2.810145	0.044144
H	7.437510	-1.509880	-1.419018
H	5.388264	0.603508	3.257803
H	4.769210	1.142693	1.703007
H	5.591767	-3.492729	0.986468
H	5.731797	-5.223173	0.540361
H	4.119402	-4.444256	0.573687
H	4.131469	-3.037362	-4.109131
H	4.813881	-1.705745	-6.081063
H	5.816050	0.559849	-5.778439
H	6.101866	1.481684	-3.502580
H	3.290588	-2.750848	-1.631649
H	4.387855	-1.898096	-0.547463
H	-4.036649	-0.291042	-0.232615
H	-1.813539	-4.171832	-2.353607
H	-3.281151	-3.403031	-3.086836
H	-1.649301	-2.738050	-3.414778
H	-8.193722	-1.139155	-5.134039
H	-8.495929	0.080590	-3.867108
H	-7.311685	0.414132	-5.182043
H	-4.497960	-5.321417	-1.013973
H	-6.892660	-5.753070	-1.478946
H	-8.583547	-3.956279	-1.113939
H	-7.850403	-1.714649	-0.366142
H	-3.234109	-2.538475	0.882929
H	-2.846008	-4.042027	0.058136
H	-7.366818	2.254136	-3.134850
H	-8.905739	3.338177	-1.534784
H	-8.914413	2.651525	0.864477
H	-7.325288	0.924072	1.647440
H	-5.331905	0.972142	-3.496917
H	-4.705295	-0.171260	-2.317749
H	-5.727898	3.853030	0.378746
H	-5.910393	5.168836	1.582092

H	-4.273467	4.591823	1.138280
H	-3.825159	1.270961	4.637467
H	-4.275473	-0.824040	5.879339
H	-5.271294	-2.787440	4.705054
H	-5.771032	-2.648079	2.289640
H	-3.244665	2.154126	2.246311
H	-4.397025	1.767570	0.970429

$[HPS_3BiCl_3I]_2$ ('e' isomer) ωB97XD/def2-SVP (PCM)

E= -8068.491180

C	-7.469162	1.143980	0.095904
C	-6.537136	0.245270	-0.432927
C	-6.442599	0.023645	-1.827099
C	-7.275051	0.782786	-2.653836
C	-8.194950	1.690541	-2.128994
C	-8.306132	1.862994	-0.752984
P	-5.409906	-0.588753	0.696665
C	-5.395990	0.115467	2.357297
C	-4.941466	1.431115	2.582147
C	-4.843980	1.871046	3.905738
C	-5.193755	1.045565	4.970475
C	-5.653857	-0.248654	4.735773
C	-5.749498	-0.716218	3.429981
C	-4.572552	2.375866	1.473099
S	-5.738267	3.783787	1.429599
C	-5.460980	4.342370	-0.266674
C	-5.520585	-0.992542	-2.454237
S	-6.257982	-2.649023	-2.676161
C	-7.453715	-2.339052	-3.994166
C	-5.815703	-2.340895	0.771308
C	-4.827114	-3.327603	0.954346
C	-5.238167	-4.662597	0.991882
C	-6.584369	-5.007974	0.881240
C	-7.553735	-4.020713	0.729235
C	-7.167211	-2.686360	0.664369
C	-3.368670	-3.003814	1.123145
S	-2.512138	-2.552919	-0.427248
C	-2.662825	-4.080938	-1.376851
Bi	0.426853	-2.258802	0.742438
Cl	-0.413263	-3.702063	2.709413
I	1.284501	-4.667550	-0.825644
I	2.965748	-1.660187	2.131275
I	1.195909	-0.334649	-1.908478
I	-1.195935	0.334761	1.908622
Bi	-0.426875	2.258813	-0.742317
I	-2.965726	1.660263	-2.131303
Cl	0.413322	3.702106	-2.709222
I	-1.284460	4.667578	0.825845
S	2.512227	2.552838	0.427369
C	2.662876	4.080791	1.377084
C	3.368683	3.003899	-1.123023
C	4.827138	3.327661	-0.954306
C	5.815721	2.340923	-0.771399
C	7.167249	2.686342	-0.664553

C	7.553795	4.020693	-0.729361
C	6.584437	5.007984	-0.881224
C	5.238218	4.662647	-0.991787
P	5.409871	0.588802	-0.696817
C	6.537146	-0.245359	0.432634
C	6.442711	-0.023857	1.826836
C	7.275180	-0.783110	2.653451
C	8.194989	-1.690872	2.128468
C	8.306063	-1.863221	0.752436
C	7.469079	-1.144085	-0.096333
C	5.520746	0.992284	2.454115
S	6.258212	2.648713	2.676225
C	7.454396	2.338385	3.993733
C	5.395763	-0.115362	-2.357460
C	5.749164	0.716330	-3.430172
C	5.653393	0.248763	-4.735954
C	5.193272	-1.045460	-4.970610
C	4.843604	-1.870943	-3.905839
C	4.941215	-1.431006	-2.582259
C	4.572407	-2.375737	-1.473156
S	5.738070	-3.783704	-1.429814
C	5.461213	-4.342092	0.266591
H	4.111322	0.446750	-0.169886
H	2.206474	4.921071	0.836681
H	3.719074	4.282711	1.603349
H	2.116692	3.915106	2.314500
H	7.899373	3.311315	4.242109
H	8.255045	1.661708	3.663131
H	6.965646	1.930708	4.890289
H	4.487185	5.444220	-1.124911
H	6.874760	6.059639	-0.919663
H	8.608681	4.285307	-0.645002
H	7.923182	1.911841	-0.517700
H	3.205107	2.143350	-1.790937
H	2.831000	3.845331	-1.579512
H	7.192451	-0.665639	3.735928
H	8.826689	-2.269883	2.804771
H	9.022742	-2.571958	0.335290
H	7.527380	-1.307676	-1.173453
H	5.174251	0.629319	3.432853
H	4.612845	1.175361	1.861150
H	5.807874	-3.585951	0.986988
H	6.043404	-5.263777	0.399584
H	4.397444	-4.558575	0.438335
H	4.478833	-2.882371	-4.098594
H	5.100092	-1.416052	-5.993234
H	5.928253	0.900472	-5.566527
H	6.091809	1.736501	-3.248256
H	3.550147	-2.755841	-1.621118
H	4.590224	-1.898017	-0.483601
H	-4.111314	-0.446640	0.169837
H	-2.206501	-4.921213	-0.836375
H	-3.719019	-4.282803	-1.603171

H	-2.116583	-3.915337	-2.314249
H	-7.898575	-3.312050	-4.242478
H	-8.254501	-1.662319	-3.664009
H	-6.964656	-1.931564	-4.890641
H	-4.487122	-5.444142	1.125110
H	-6.874671	-6.059634	0.919723
H	-8.608610	-4.285354	0.644820
H	-7.923154	-1.911888	0.517406
H	-3.205175	-2.143208	1.790997
H	-2.831031	-3.845197	1.579775
H	-7.192244	0.665226	-3.736297
H	-8.826637	2.269455	-2.805392
H	-9.022885	2.571719	-0.335945
H	-7.527533	1.307672	1.173005
H	-5.174064	-0.629675	-3.433003
H	-4.612692	-1.175516	-1.861222
H	-5.807522	3.586341	-0.987244
H	-6.043071	5.264114	-0.399693
H	-4.397155	4.558788	-0.438150
H	-4.479218	2.882470	4.098528
H	-5.100671	1.416152	5.993110
H	-5.928796	-0.900359	5.566322
H	-6.092121	-1.736390	3.248034
H	-3.550338	2.756038	1.621192
H	-4.590177	1.898150	0.483545

[$HPS_3BiCl_3I]_2$ ('f' isomer) ωB97XD/def2-SVP (PCM)

E= -8068.497649

C	7.383176	1.110655	-0.071450
C	6.349292	0.433578	0.583483
C	6.143700	0.578010	1.975256
C	6.971200	1.476185	2.654466
C	7.995201	2.161963	2.001029
C	8.216604	1.968206	0.641445
P	5.271283	-0.625848	-0.392423
C	5.411323	-0.333635	-2.166845
C	4.980361	0.882724	-2.736196
C	5.035940	1.005687	-4.128162
C	5.511996	-0.028090	-4.929591
C	5.945874	-1.220910	-4.354485
C	5.890074	-1.375838	-2.974047
C	4.493707	2.051291	-1.924834
S	5.728414	3.403790	-1.954840
C	5.425757	4.148515	-0.334377
C	5.119549	-0.206250	2.757018
S	5.747030	-1.778399	3.444578
C	6.867069	-1.189203	4.733732
C	5.645265	-2.350534	-0.026930
C	4.662254	-3.357965	-0.081602
C	5.050366	-4.666689	0.216089
C	6.373114	-4.975397	0.529746
C	7.340231	-3.974890	0.556331
C	6.973031	-2.660511	0.287205
C	3.227883	-3.085882	-0.441241

S	2.263660	-2.284545	0.887931
C	2.391050	-3.500958	2.215538
Bi	-0.612141	-2.307830	-0.381822
I	0.189922	-4.172459	-2.576300
I	-1.331940	-4.518980	1.465830
Cl	-2.981566	-1.927564	-1.381240
I	-1.081200	-0.094117	1.990151
I	1.081172	0.094114	-1.990114
Bi	0.612105	2.307832	0.381817
Cl	2.981560	1.927343	1.381162
I	-0.189776	4.172432	2.576255
I	1.332101	4.518915	-1.465798
S	-2.263619	2.284740	-0.887774
C	-2.391090	3.501449	-2.215107
C	-3.227941	3.085609	0.441610
C	-4.662287	3.357850	0.081973
C	-5.645374	2.350493	0.027102
C	-6.973112	2.660599	-0.286997
C	-7.340231	3.975053	-0.555880
C	-6.373062	4.975497	-0.529049
C	-5.050329	4.666660	-0.215433
P	-5.271463	0.625759	0.392427
C	-6.349318	-0.433546	-0.583770
C	-6.143466	-0.577677	-1.975520
C	-6.970689	-1.475886	-2.655045
C	-7.994721	-2.161899	-2.001912
C	-8.216430	-1.968370	-0.642340
C	-7.383249	-1.110843	0.070866
C	-5.119280	0.206867	-2.756961
S	-5.746799	1.779222	-3.444013
C	-6.867125	1.190525	-4.733138
C	-5.411657	0.333315	2.166800
C	-5.890491	1.375386	2.974123
C	-5.946364	1.220250	4.354533
C	-5.512469	0.027363	4.929495
C	-5.036328	-1.006284	4.127952
C	-4.980691	-0.883111	2.736007
C	-4.493955	-2.051519	1.924488
S	-5.728470	-3.404174	1.954444
C	-5.426032	-4.148512	0.333779
H	-3.944092	0.349449	0.014255
H	-2.045677	4.486683	-1.874372
H	-3.423392	3.549631	-2.588202
H	-1.730075	3.146250	-3.016309
H	-7.221381	2.082996	-5.266386
H	-7.736043	0.668331	-4.308347
H	-6.345496	0.534451	-5.444705
H	-4.300496	5.459977	-0.187649
H	-6.646066	6.009006	-0.750288
H	-8.377694	4.210308	-0.797485
H	-7.725269	1.870515	-0.334764
H	-3.131543	2.404868	1.302462
H	-2.721494	4.018140	0.724893

H	-6.805509	-1.644214	-3.721153
H	-8.623238	-2.853581	-2.566095
H	-9.017471	-2.500064	-0.126912
H	-7.527698	-0.988273	1.145204
H	-4.724885	-0.406833	-3.579260
H	-4.247062	0.495390	-2.153851
H	-5.642784	-3.430501	-0.470356
H	-6.109294	-5.004491	0.249972
H	-4.388629	-4.498649	0.244486
H	-4.692836	-1.935469	4.588414
H	-5.541206	-0.099383	6.013422
H	-6.318246	2.034594	4.977956
H	-6.214172	2.316089	2.525131
H	-3.540848	-2.420820	2.330671
H	-4.303121	-1.799648	0.871927
H	3.943936	-0.349464	-0.014213
H	2.045687	-4.486265	1.874958
H	3.423330	-3.549039	2.588694
H	1.729966	-3.145641	3.016631
H	7.221683	-2.081509	5.267023
H	7.735777	-0.666640	4.308973
H	6.345106	-0.533349	5.445256
H	4.300551	-5.460032	0.188523
H	6.646166	-6.008842	0.751225
H	8.377714	-4.210027	0.797963
H	7.725159	-1.870395	0.334832
H	3.131389	-2.405443	-1.302312
H	2.721486	-4.018555	-0.724173
H	6.806278	1.644659	3.720591
H	8.623936	2.853627	2.564992
H	9.017622	2.499697	0.125774
H	7.527442	0.987869	-1.145788
H	4.725287	0.407688	3.579203
H	4.247252	-0.494898	2.154095
H	5.641923	3.430573	0.469967
H	6.109204	5.004332	-0.250470
H	4.388437	4.499024	-0.245636
H	4.692456	1.934817	-4.588744
H	5.540683	0.098509	-6.013537
H	6.317685	-2.035364	-4.977807
H	6.213749	-2.316487	-2.524940
H	3.540729	2.420683	-2.331255
H	4.302620	1.799498	-0.872291

[$HPS_3BiCl_3I]_2$ ('g' isomer) ωB97XD/def2-SVP (PCM)

E= -8068.490526

C	-4.842084	-0.699771	3.018494
C	-5.376725	0.421206	2.349106
C	-5.806758	1.547398	3.066872
C	-5.708889	1.572041	4.453352
C	-5.171489	0.475228	5.123896
C	-4.747141	-0.643247	4.412631
P	-5.402092	0.513392	0.546197
C	-6.463499	-0.710293	-0.239154

C	-6.392326	-0.914871	-1.637372
C	-7.164323	-1.949250	-2.172925
C	-8.000688	-2.726390	-1.371929
C	-8.086790	-2.486818	-0.004198
C	-7.311216	-1.479813	0.563689
C	-5.544303	-0.079456	-2.565495
S	-6.404814	1.340293	-3.326089
C	-7.480111	0.509342	-4.517019
C	-4.380647	-1.942501	2.309032
S	-5.416312	-3.367504	2.793055
C	-4.836019	-4.560385	1.564251
C	-5.904712	2.159946	0.018185
C	-4.971525	3.196074	-0.181207
C	-5.455238	4.435710	-0.608174
C	-6.818689	4.652762	-0.800930
C	-7.733161	3.629235	-0.569762
C	-7.273639	2.378549	-0.171007
C	-3.498374	3.031736	0.069749
S	-2.585759	2.159469	-1.251915
C	-2.706669	3.341450	-2.611538
Bi	0.381337	2.393240	-0.124579
Cl	1.064017	3.798025	-2.204872
I	-1.163578	0.298344	1.930607
I	2.929203	2.347707	1.365528
I	-0.456943	4.838236	1.370431
I	1.163780	-0.298411	-1.930662
Bi	-0.381345	-2.393205	0.124296
I	-2.929268	-2.347473	-1.365723
I	0.457019	-4.837915	-1.371141
Cl	-1.064074	-3.798302	2.204398
S	2.585504	-2.159439	1.251872
C	2.706141	-3.341211	2.611706
C	3.498360	-3.031907	-0.069484
C	4.971477	-3.196185	0.181740
C	5.904685	-2.160066	-0.017602
C	7.273586	-2.378645	0.171805
C	7.733059	-3.629288	0.570748
C	6.818560	-4.652798	0.801887
C	5.455138	-4.435774	0.608904
P	5.402145	-0.513553	-0.545822
C	5.377048	-0.421525	-2.348745
C	4.842446	0.699355	-3.018331
C	4.747730	0.642683	-4.412479
C	5.172260	-0.475834	-5.123566
C	5.709617	-1.572547	-4.452826
C	5.807261	-1.547761	-3.066333
C	4.380799	1.942143	-2.309097
S	5.416478	3.367145	-2.793096
C	4.834984	4.560541	-1.565364
C	6.463475	0.710182	0.239566
C	7.311290	1.479619	-0.563255
C	8.086830	2.486657	0.004621
C	8.000595	2.726348	1.372322

C	7.164140	1.949288	2.173298
C	6.392183	0.914869	1.637763
C	5.544077	0.079553	2.565899
S	6.404533	-1.340028	3.326868
C	7.479464	-0.508876	4.517983
H	-4.089536	0.274534	0.093729
H	-2.249489	4.299942	-2.331434
H	-3.756070	3.474679	-2.907752
H	-2.145127	2.905301	-3.447383
H	-7.957829	1.301891	-5.108760
H	-8.265431	-0.076440	-4.018676
H	-6.899998	-0.137204	-5.191138
H	-4.747537	5.250965	-0.774104
H	-7.166965	5.633883	-1.129408
H	-8.801332	3.795338	-0.715217
H	-7.987117	1.565629	-0.018876
H	-3.290151	2.451720	0.982810
H	-3.028321	4.012800	0.216993
H	-7.096054	-2.159481	-3.242312
H	-8.584744	-3.529938	-1.824680
H	-8.736203	-3.092952	0.628837
H	-7.352404	-1.313870	1.641232
H	-5.142816	-0.710314	-3.371999
H	-4.670527	0.365417	-2.067756
H	-5.132585	-4.252217	0.551030
H	-5.305568	-5.523996	1.802809
H	-3.742631	-4.662140	1.614945
H	-4.325271	-1.498922	4.944281
H	-5.076130	0.491813	6.211271
H	-6.042574	2.452300	5.004603
H	-6.210884	2.415326	2.543171
H	-3.331020	-2.162876	2.559328
H	-4.429378	-1.845802	1.215074
H	4.089514	-0.274645	-0.093587
H	2.249057	-4.299759	2.331647
H	3.755479	-3.474364	2.908179
H	2.144410	-2.904941	3.447360
H	7.957044	-1.301335	5.109956
H	8.264901	0.076867	4.019780
H	6.899147	0.137735	5.191865
H	4.747419	-5.251020	0.774796
H	7.166794	-5.633883	1.130516
H	8.801211	-3.795372	0.716369
H	7.987083	-1.565737	0.019696
H	3.290294	-2.452038	-0.982671
H	3.028363	-4.013008	-0.216655
H	7.095772	2.159609	3.242662
H	8.584623	3.529920	1.825066
H	8.736308	3.092729	-0.628406
H	7.352586	1.313585	-1.640780
H	5.142432	0.710533	3.372230
H	4.670403	-0.365453	2.068101
H	5.131054	4.253100	-0.551777

H	5.304308	5.524186	-1.804226
H	3.741586	4.661844	-1.616766
H	4.325894	1.498282	-4.944280
H	5.077073	-0.492535	-6.210954
H	6.043442	-2.452844	-5.003932
H	6.211360	-2.415612	-2.542485
H	3.331219	2.162435	-2.559659
H	4.429272	1.845584	-1.215116

[$HPS_3BiCl_3I]_2$ ('h' isomer) ωB97XD/def2-SVP (PCM)

E = -8068.495034

C	-4.647879	-1.061683	3.033917
C	-5.163712	0.158684	2.550601
C	-5.505632	1.193359	3.434074
C	-5.338756	1.026316	4.803863
C	-4.819050	-0.171000	5.291818
C	-4.480221	-1.197816	4.415688
P	-5.278308	0.488386	0.780049
C	-6.429189	-0.587577	-0.091066
C	-6.434667	-0.626919	-1.505206
C	-7.274403	-1.562059	-2.115995
C	-8.105190	-2.395659	-1.367349
C	-8.116483	-2.315312	0.021517
C	-7.270700	-1.413274	0.660698
C	-5.602613	0.287092	-2.370764
S	-6.447261	1.820419	-2.892775
C	-7.626028	1.186193	-4.106585
C	-4.284634	-2.216562	2.142691
S	-5.367344	-3.646112	2.495427
C	-4.961598	-4.661956	1.055334
C	-5.736937	2.207808	0.506032
C	-4.775030	3.234431	0.430696
C	-5.229107	4.538771	0.218864
C	-6.589881	4.823190	0.113366
C	-7.531160	3.803309	0.216301
C	-7.102756	2.492993	0.402184
C	-3.299307	2.989640	0.583971
S	-2.494253	2.254735	-0.882603
C	-2.754328	3.546731	-2.117156
Bi	0.571790	2.236167	0.073490
I	1.254713	4.143924	-2.103727
I	-0.992226	-0.023054	1.939369
Cl	2.918043	1.979003	1.139126
I	-0.052385	4.416464	2.013898
I	1.254858	-0.234293	-1.998823
Bi	-0.419158	-2.478773	-0.225418
I	-2.994172	-2.221331	-1.669584
I	0.532932	-4.690529	-1.978620
Cl	-1.140261	-4.138327	1.644438
S	2.373215	-2.285845	1.150098
C	2.340856	-3.459542	2.521019
C	3.456297	-3.140902	-0.047008
C	4.869647	-3.316934	0.434314
C	5.811233	-2.269332	0.442980

C	7.121991	-2.486941	0.881415
C	7.512595	-3.747430	1.321194
C	6.584860	-4.784868	1.339527
C	5.279299	-4.568550	0.901406
P	5.402601	-0.613143	-0.137746
C	5.688478	-0.497193	-1.915577
C	5.261210	0.631662	-2.645550
C	5.445897	0.619303	-4.031837
C	6.044213	-0.461082	-4.674084
C	6.471411	-1.566457	-3.940770
C	6.288861	-1.586978	-2.562724
C	4.641511	1.842238	-2.004597
S	5.776249	3.274823	-2.116751
C	5.268561	4.195571	-0.644832
C	6.343024	0.597317	0.804980
C	7.377543	1.283036	0.160398
C	8.098694	2.258513	0.843216
C	7.768007	2.555228	2.161565
C	6.742754	1.862419	2.805539
C	6.022722	0.854759	2.158214
C	4.974816	0.090741	2.928991
S	5.608987	-1.363764	3.833539
C	6.540751	-0.578130	5.167131
H	-4.001294	0.266585	0.228538
H	-2.316529	4.496549	-1.781503
H	-3.826604	3.660577	-2.328777
H	-2.238240	3.212282	-3.026170
H	-8.114144	2.064147	-4.550826
H	-8.395769	0.558218	-3.636451
H	-7.116259	0.623488	-4.901903
H	-4.499170	5.348360	0.151260
H	-6.913481	5.853383	-0.046474
H	-8.597145	4.019976	0.135274
H	-7.838734	1.687759	0.454492
H	-3.072807	2.289019	1.403342
H	-2.782766	3.927396	0.827739
H	-7.266891	-1.648257	-3.204604
H	-8.745578	-3.116515	-1.879240
H	-8.762086	-2.965182	0.613704
H	-7.250267	-1.374200	1.750785
H	-5.270208	-0.248489	-3.271770
H	-4.687271	0.635284	-1.870788
H	-5.333601	-4.193777	0.132139
H	-5.455441	-5.632850	1.195132
H	-3.874796	-4.810714	0.984716
H	-4.071576	-2.132700	4.805719
H	-4.671614	-0.306748	6.364842
H	-5.606900	1.834256	5.486017
H	-5.898309	2.137079	3.051470
H	-3.238210	-2.516074	2.305886
H	-4.382208	-1.976188	1.074163
H	4.036641	-0.363836	0.095444
H	1.964459	-4.434652	2.184253

H	3.339692	-3.549505	2.969314
H	1.644311	-3.043454	3.259975
H	6.884327	-1.387526	5.825402
H	7.419851	-0.039816	4.785725
H	5.904488	0.105112	5.747941
H	4.561224	-5.391404	0.909697
H	6.876688	-5.774814	1.695250
H	8.535948	-3.911321	1.661513
H	7.842473	-1.666288	0.892179
H	3.392406	-2.535323	-0.965094
H	3.006396	-4.113358	-0.287175
H	6.489676	2.113921	3.837570
H	8.308800	3.337146	2.698347
H	8.899034	2.797482	0.334289
H	7.607914	1.075163	-0.885473
H	4.473482	0.760181	3.642548
H	4.178850	-0.310389	2.286480
H	5.486612	3.623586	0.268958
H	5.851438	5.126613	-0.639531
H	4.197322	4.437160	-0.680762
H	5.109180	1.479175	-4.615549
H	6.173832	-0.440671	-5.757865
H	6.937978	-2.417612	-4.438716
H	6.607793	-2.460498	-1.991303
H	3.690666	2.087109	-2.500778
H	4.404747	1.689773	-0.943083

[$HPS_3BiCl_3I]_2$ ('i' isomer) ωB97XD/def2-SVP (PCM)

E= -8068.494352

C	-4.777746	-1.278612	2.623728
C	-5.201322	0.028890	2.309140
C	-5.500390	0.951077	3.322532
C	-5.378615	0.583928	4.657817
C	-4.947966	-0.701514	4.980534
C	-4.653935	-1.617627	3.974689
P	-5.227591	0.609330	0.601939
C	-6.391671	-0.268055	-0.453960
C	-6.309064	-0.140565	-1.860343
C	-7.174060	-0.926468	-2.626665
C	-8.113613	-1.768941	-2.032796
C	-8.212760	-1.846390	-0.647034
C	-7.344728	-1.098838	0.144016
C	-5.367257	0.806852	-2.561924
S	-6.071985	2.458045	-2.902157
C	-7.232747	2.080940	-4.233850
C	-4.472142	-2.317517	1.581319
S	-5.689690	-3.677186	1.681815
C	-5.482161	-4.385514	0.031426
C	-5.590419	2.372393	0.554058
C	-4.579507	3.346621	0.670368
C	-4.959507	4.690118	0.616328
C	-6.297607	5.058328	0.481825
C	-7.289311	4.085713	0.395581
C	-6.933366	2.741437	0.421098

C	-3.128289	3.002556	0.862721
S	-2.281478	2.416530	-0.647175
C	-2.450737	3.848644	-1.733458
Bi	0.702211	2.146804	0.434440
I	1.449472	4.455105	-1.294514
I	-1.020042	-0.325919	1.853430
Cl	3.061422	1.636826	1.382765
I	0.071405	3.894865	2.770845
I	1.219884	0.091295	-2.083254
Bi	-0.394374	-2.436258	-0.664217
I	-2.933928	-1.959879	-2.113735
Cl	0.565129	-4.002306	-2.483550
I	-1.263624	-4.738560	1.023031
S	2.445839	-2.451573	0.658915
C	2.550035	-3.792467	1.863221
C	3.407663	-3.132002	-0.738534
C	4.840586	-3.436056	-0.401040
C	5.826271	-2.437774	-0.275018
C	7.153200	-2.771056	0.017805
C	7.516586	-4.102108	0.195232
C	6.547090	-5.096077	0.096711
C	5.225344	-4.763710	-0.196934
P	5.448099	-0.693404	-0.520874
C	5.593393	-0.272313	-2.268692
C	5.146716	0.976155	-2.750447
C	5.219488	1.205952	-4.127992
C	5.727413	0.245400	-4.998162
C	6.175377	-0.980103	-4.508713
C	6.103003	-1.241181	-3.145141
C	4.621146	2.067182	-1.859787
S	5.827322	3.441496	-1.737702
C	5.487821	4.010505	-0.054593
C	6.517134	0.304605	0.526533
C	7.547755	1.030922	-0.079056
C	8.375330	1.841943	0.692423
C	8.150405	1.941663	2.061655
C	7.128352	1.208582	2.665077
C	6.307598	0.353758	1.924320
C	5.284201	-0.487858	2.644578
S	5.917744	-2.097103	3.232747
C	6.981693	-1.591199	4.602268
H	-3.939467	0.398380	0.072520
H	-2.006631	4.741218	-1.272783
H	-3.509046	4.015370	-1.977936
H	-1.900110	3.604493	-2.651029
H	-7.630972	3.043872	-4.581305
H	-8.070382	1.463035	-3.880710
H	-6.726770	1.582284	-5.073103
H	-4.190931	5.461918	0.695626
H	-6.563069	6.116631	0.447244
H	-8.337764	4.368127	0.291346
H	-7.706518	1.976342	0.323400
H	-2.983897	2.191117	1.594091

H	-2.580542	3.870639	1.253218
H	-7.102282	-0.882574	-3.715452
H	-8.770388	-2.371772	-2.662848
H	-8.945138	-2.503571	-0.176257
H	-7.394650	-1.189715	1.230141
H	-5.034939	0.369554	-3.514637
H	-4.451637	1.010361	-1.987808
H	-5.820575	-3.677268	-0.739661
H	-6.104128	-5.289895	-0.008801
H	-4.432999	-4.658668	-0.149017
H	-4.313388	-2.622158	4.236020
H	-4.834057	-0.992761	6.026416
H	-5.610089	1.306173	5.441821
H	-5.819275	1.964206	3.070963
H	-3.460460	-2.723447	1.732489
H	-4.500591	-1.914756	0.558839
H	4.119069	-0.452295	-0.125636
H	2.163315	-4.728101	1.437801
H	3.586271	-3.912060	2.208139
H	1.918387	-3.491543	2.709074
H	7.333345	-2.515947	5.079326
H	7.855913	-1.024757	4.251316
H	6.423189	-0.999595	5.341764
H	4.473804	-5.551570	-0.281275
H	6.817667	-6.142839	0.247067
H	8.552988	-4.356347	0.421678
H	7.907007	-1.987539	0.120021
H	3.311565	-2.374817	-1.532900
H	2.893169	-4.028130	-1.109727
H	6.959362	1.305737	3.739442
H	8.774434	2.597088	2.672266
H	9.174369	2.411461	0.215900
H	7.694715	0.981890	-1.158906
H	4.876228	0.066392	3.501779
H	4.420495	-0.744371	2.015468
H	5.760797	3.240679	0.681512
H	6.106904	4.903293	0.107082
H	4.428621	4.275220	0.066719
H	4.863362	2.160623	-4.522263
H	5.769314	0.453902	-6.068931
H	6.570633	-1.737696	-5.186927
H	6.438406	-2.207330	-2.763601
H	3.672620	2.454567	-2.259634
H	4.405332	1.725167	-0.838335

$[HPS_3BiCl_3I]_2$ ('j' isomer) ωB97XD/def2-SVP (PCM)

E = -8068.491132

C	-5.863894	-1.357744	-2.917202
C	-5.444187	-0.316706	-2.075972
C	-5.005161	0.911674	-2.612196
C	-4.988796	1.048079	-4.003666
C	-5.403254	0.014121	-4.838171
C	-5.849474	-1.189916	-4.297105
P	-5.347895	-0.647022	-0.304830

C	-6.408300	0.407685	0.695614
C	-6.231650	0.473219	2.097842
C	-7.024218	1.385043	2.800398
C	-7.982488	2.167570	2.156051
C	-8.173192	2.057610	0.782431
C	-7.378580	1.180261	0.049661
C	-5.262664	-0.393423	2.864549
S	-5.962991	-1.964567	3.479138
C	-7.091046	-1.376720	4.762012
C	-4.581827	2.080198	-1.766164
S	-5.774335	3.451295	-1.971467
C	-5.393117	4.404111	-0.483555
C	-5.742832	-2.372288	0.024309
C	-4.759296	-3.379486	-0.014144
C	-5.156332	-4.690686	0.260136
C	-6.488020	-4.999216	0.534639
C	-7.455033	-3.998079	0.542417
C	-7.079456	-2.681323	0.298003
C	-3.321992	-3.101952	-0.355182
S	-2.345211	-2.366427	1.002592
C	-2.325036	-3.713187	2.204199
Bi	0.504707	-2.319883	-0.329144
I	3.091589	-1.930237	-1.721332
I	1.134922	-0.030322	1.994673
Bi	-0.353822	2.425323	0.320090
Cl	0.505880	4.235846	1.954803
I	-1.194174	4.454289	-1.693220
I	-2.869562	2.191919	1.830056
I	-0.338892	-4.398361	-2.295605
Cl	1.225410	-4.124423	1.409526
I	-1.211625	0.033724	-1.895884
S	2.692019	2.410512	-0.701525
C	2.940985	3.815946	-1.807902
C	3.478551	3.021504	0.830842
C	4.955701	3.273419	0.715291
C	5.913003	2.240163	0.737963
C	7.281414	2.524576	0.674589
C	7.716658	3.842552	0.582051
C	6.780410	4.871240	0.531468
C	5.417052	4.586979	0.597189
P	5.435674	0.510814	0.889803
C	5.284137	0.065180	2.631913
C	4.746013	-1.178595	3.021994
C	4.551989	-1.406728	4.387950
C	4.884574	-0.445363	5.337648
C	5.425096	0.776435	4.941344
C	5.619658	1.033867	3.589331
C	4.383352	-2.263207	2.046612
S	5.452795	-3.721634	2.303622
C	5.056092	-4.626723	0.789233
C	6.595388	-0.514933	-0.028378
C	6.625725	-0.459024	-1.441579
C	7.475202	-1.352576	-2.099429

C	8.292913	-2.235221	-1.393812
C	8.278887	-2.249289	-0.002773
C	7.422073	-1.391465	0.681282
C	5.807215	0.511496	-2.257593
S	6.661018	2.072417	-2.671711
C	7.840599	1.512423	-3.920577
H	-4.017228	-0.404450	0.089331
H	-1.890535	-4.618093	1.759189
H	-3.338599	-3.901071	2.583696
H	-1.681371	-3.376715	3.026800
H	-7.495238	-2.272571	5.252360
H	-7.926847	-0.803509	4.336452
H	-6.562361	-0.769507	5.510841
H	-4.408308	-5.486012	0.240054
H	-6.768968	-6.034332	0.737609
H	-8.499072	-4.234799	0.751918
H	-7.831088	-1.889835	0.332827
H	-3.219868	-2.386952	-1.187190
H	-2.821030	-4.023874	-0.678781
H	-6.879821	1.491269	3.877576
H	-8.582929	2.869529	2.737780
H	-8.920930	2.666309	0.272265
H	-7.501538	1.119245	-1.032641
H	-4.858447	0.165120	3.721271
H	-4.392738	-0.700965	2.266157
H	-5.686008	3.849149	0.420298
H	-5.973392	5.334786	-0.541709
H	-4.322213	4.647952	-0.438076
H	-4.637568	1.987684	-4.436056
H	-5.372966	0.149714	-5.920925
H	-6.175783	-2.003534	-4.946388
H	-6.195538	-2.308139	-2.495437
H	-3.577092	2.421198	-2.059970
H	-4.528443	1.835404	-0.695897
H	4.168243	0.337199	0.299205
H	2.491753	4.724386	-1.383970
H	4.012577	3.961847	-2.002227
H	2.432820	3.564770	-2.747681
H	8.333330	2.414492	-4.307740
H	8.606882	0.852130	-3.490623
H	7.329983	1.003310	-4.750863
H	4.690715	5.402126	0.572309
H	7.110641	5.908056	0.443898
H	8.784516	4.059696	0.532464
H	8.013512	1.714211	0.684650
H	3.241836	2.257180	1.587653
H	2.949337	3.930960	1.143426
H	7.487052	-1.365423	-3.191287
H	8.942433	-2.920330	-1.941965
H	8.913987	-2.938424	0.555408
H	7.380693	-1.428086	1.770859
H	5.485860	0.035364	-3.195330
H	4.885877	0.829336	-1.748268

H	5.438334	-4.093843	-0.093932
H	5.544913	-5.607412	0.861957
H	3.969311	-4.764844	0.698742
H	4.125648	-2.360840	4.705630
H	4.715570	-0.650403	6.396443
H	5.687500	1.534043	5.680954
H	6.027926	1.997411	3.279489
H	3.333419	-2.565504	2.179313
H	4.489708	-1.945222	0.999316

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