

## Supplementary Information for

# Evaluation of bismuth-based dispersion energy donors – synthesis, structure and theoretical study of 2-biphenylbismuth(III) derivatives

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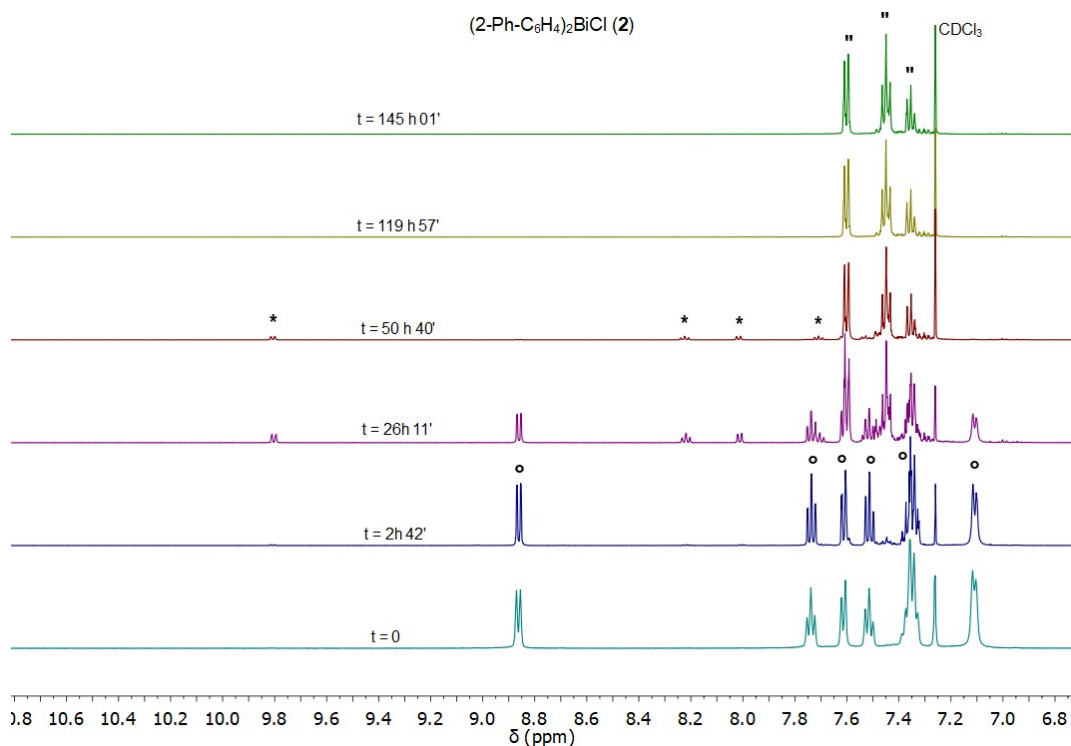
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**Table S1** Crystallographic data and structure refinement details for (2-PhC<sub>6</sub>H<sub>4</sub>)<sub>3</sub>Bi (**1**), (2-PhC<sub>6</sub>H<sub>4</sub>)<sub>2</sub>BiCl (**2**), (2-PhC<sub>6</sub>H<sub>4</sub>)<sub>2</sub>BiBr (**3**), (2-PhC<sub>6</sub>H<sub>4</sub>)<sub>2</sub>BiI (**4**), (2-PhC<sub>6</sub>H<sub>4</sub>)<sub>2</sub>BiMe (**5**) and Bi(2-PhC<sub>6</sub>H<sub>4</sub>)BiCl<sub>2</sub> (**6**).

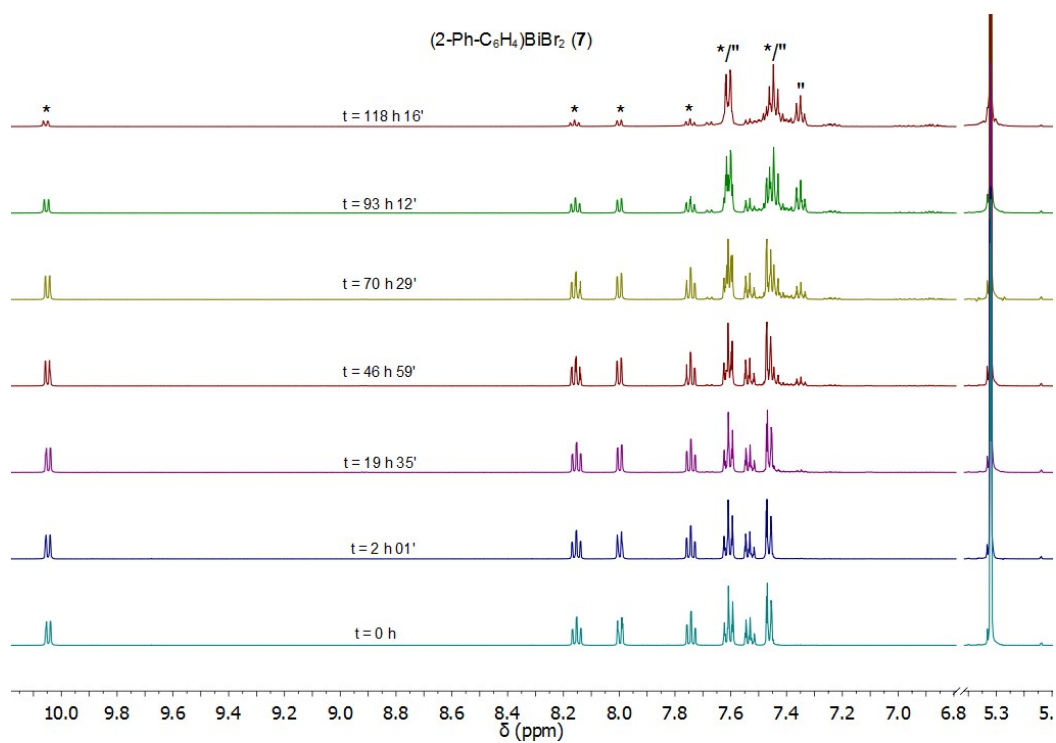
	<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>	<b>5</b>	<b>6</b>
Empirical formula	C <sub>36</sub> H <sub>27</sub> Bi	C <sub>24</sub> H <sub>18</sub> BiCl	C <sub>24</sub> H <sub>18</sub> BiBr	C <sub>24</sub> H <sub>18</sub> BiI	C <sub>25</sub> H <sub>21</sub> Bi	C <sub>12</sub> H <sub>9</sub> BiCl <sub>2</sub>
<i>M</i> (g mol <sup>-1</sup> )	668.55	550.81	595.27	642.26	530.40	433.07
Temperature (K)	120	100	116	100	100	100
$\lambda$ (Å)	1.54184	1.54178	0.71073	0.71073	1.54178	0.71073
Crystal system	monoclinic	triclinic	monoclinic	triclinic	monoclinic	orthorhombic
Space group	<i>P</i> 2 <sub>1</sub> / <i>n</i>	<i>P</i> $\bar{1}$	<i>P</i> 2 <sub>1</sub> / <i>n</i>	<i>P</i> $\bar{1}$	<i>P</i> 2 <sub>1</sub>	<i>P</i> 2 <sub>1</sub> 2 <sub>1</sub>
<i>a</i> (Å)	10.0767(1)	9.9371(3)	9.9115(7)	9.3194(9)	15.1772(5)	7.6237(7)
<i>b</i> (Å)	20.4313(1)	11.3295(4)	15.7922(9)	9.6034(9)	6.7889(3)	9.0462(8)
<i>c</i> (Å)	13.8429(1)	17.9137(6)	13.3369(8)	12.8339(12)	19.2090(7)	17.6540(17)
$\alpha$ (deg)	90	78.588(1)	90	108.743(3)	90	90
$\beta$ (deg)	109.817(1)	86.690(1)	107.717(7)	99.713(3)	99.773(3)	90
$\gamma$ (deg)	90	78.695(1)	90	103.712(3)	90	90
<i>V</i> (Å <sup>3</sup> )	2681.20(4)	1938.16(11)	1988.5(2)	1018.57(17)	1950.51(13)	1217.52(19)
<i>Z</i>	4	4	4	2	4	4
<i>D</i> <sub>calc</sub> (g cm <sup>-3</sup> )	1.656	1.888	1.988	2.097	1.806	2.363
$\mu$ (mm <sup>-1</sup> )	13.062	19.133	10.880	10.174	17.710	14.883
<i>F</i> (000)	1304	1048	1120	598	1016	792
Crystal size (mm)	0.2 x 0.2 x 0.1	0.27 x 0.12 x 0.12	0.4 x 0.4 x 0.4	0.42 x 0.35 x 0.31	0.45 x 0.09 x 0.06	0.1 x 0.1 x 0.1
Reflections collected	23124	26560	8769	15873	28460	5829
Independent reflections	4819	6656	3653	3558	6360	2249
<i>R</i> <sub>int</sub>	0.0384	0.0351	0.0318	0.0443	0.0566	0.0385
Number of data / restraints / parameters	4819 / 0 / 334	6656 / 0 / 470	3653 / 0 / 235	3558 / 0 / 235	6360 / 37 / 469	2249 / 111 / 138
Goodness-of-fit on <i>F</i> <sup>2</sup>	1.082	1.090	1.041	1.087	1.102	0.801
Final <i>R</i> indices [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )]						
<i>R</i> <sub>1</sub>	0.0235	0.0210	0.0310	0.0526	0.0533	0.0204
<i>wR</i> <sub>2</sub>	0.0568	0.0521	0.0624	0.1411	0.1422	0.0449
<i>R</i> indices (all data)						
<i>R</i> <sub>1</sub>	0.0269	0.0222	0.0447	0.0545	0.0591	0.0224
<i>wR</i> <sub>2</sub>	0.0586	0.0528	0.0675	0.1427	0.11489	0.0457
Flack <i>x</i> parameter <sup>1</sup>					-0.059(12)	0.021(11)
$\Delta\rho$ <sub>min</sub> and $\Delta\rho$ <sub>max</sub> (e Å <sup>-3</sup> )	-0.745 and 0.914	-1.224 and 1.026	-1.715 and 1.212	-1.012 and 4.718	-1.542 and 4.754	-0.785 and 1.000

**Table S2** Crystallographic data and structure refinement details for (2-PhC<sub>6</sub>H<sub>4</sub>)BiBr<sub>2</sub> (**7**), (2-PhC<sub>6</sub>H<sub>4</sub>)BiI<sub>2</sub> (**8**) and (2-PhC<sub>6</sub>H<sub>4</sub>)<sub>3</sub>Sb (**9**).

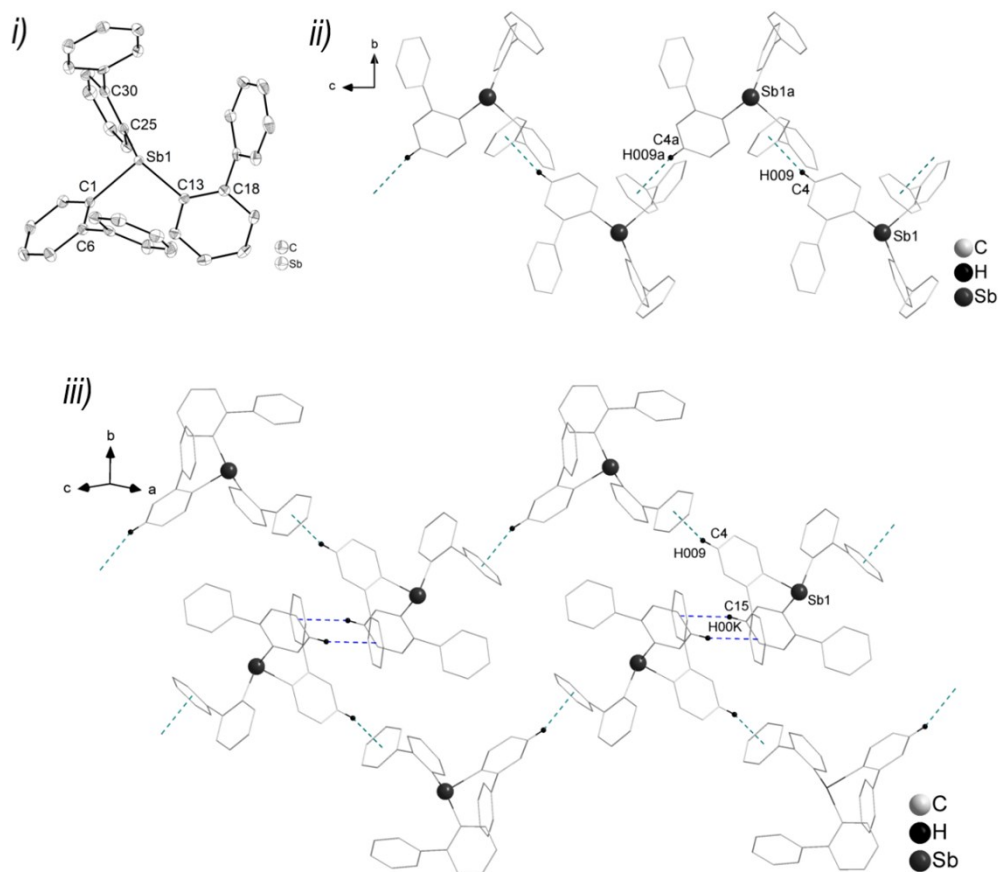
	<b>7</b>	<b>8</b>	<b>9</b>
Empirical formula	C <sub>12</sub> H <sub>9</sub> BiBr <sub>2</sub>	C <sub>24</sub> H <sub>18</sub> Bi <sub>2</sub> I <sub>4</sub>	C <sub>36</sub> H <sub>27</sub> Sb
<i>M</i> (g mol <sup>-1</sup> )	521.99	1231.94	581.32
Temperature (K)	293	100	100
$\lambda$ (Å)	0.71073 Å	0.71073	0.71073
Crystal system	monoclinic	triclinic	monoclinic
Space group	<i>P</i> 2 <sub>1</sub> / <i>c</i>	<i>P</i> $\bar{1}$	<i>P</i> 2 <sub>1</sub> / <i>n</i>
<i>a</i> (Å)	7.5467(5)	9.4889(9)	10.0086(7)
<i>b</i> (Å)	9.2977(5)	9.9731(9)	20.2781(14)
<i>c</i> (Å)	18.6372(12)	14.6288(13)	13.7772(10)
$\alpha$ (deg)	90	102.420(3)	90
$\beta$ (deg)	94.936(6)	93.506(3)	109.442(2)
$\gamma$ (deg)	90	92.701(3)	90
<i>V</i> (Å <sup>3</sup> )	1302.87(14)	1346.9(2)	2636.7(3)
<i>Z</i>	4	2	4
<i>D</i> <sub>calc</sub> (g cm <sup>-3</sup> )	2.661	3.038	1.464
$\mu$ (mm <sup>-1</sup> )	19.632	17.642	1.070
<i>F</i> (000)	936	1080	1176
Crystal size (mm)	0.4 x 0.4 x 0.4	0.4 x 0.4 x 0.3	0.35 x 0.3 x 0.3
Reflections collected	8056	33289	27264
Independent reflections	2349	5105	4957
<i>R</i> <sub>int</sub>	0.0597	0.0439	0.0301
Number of data / restraints / parameters	2349 / 194 / 192	5105 / 0 / 272	4957 / 0 / 335
Goodness-of-fit on <i>F</i> <sup>2</sup>	1.076	1.131	1.045
Final <i>R</i> indices [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )]			
<i>R</i> <sub>1</sub>	0.0390	0.0241	0.0187
<i>wR</i> <sub>2</sub>	0.0936	0.0601	0.0469
<i>R</i> indices (all data)			
<i>R</i> <sub>1</sub>	0.0536	0.0253	0.0205
<i>wR</i> <sub>2</sub>	0.1030	0.0609	0.0481
$\Delta\rho$ <sub>min</sub> and $\Delta\rho$ <sub>max</sub> (e Å <sup>-3</sup> )	-1.090 and 1.490	-1.828 and 1.686	-0.431 and 0.485



**Figure S1.** Time dependent <sup>1</sup>H NMR spectra of the stability of (2-Ph-C<sub>6</sub>H<sub>4</sub>)<sub>2</sub>BiCl (**2**) in CDCl<sub>3</sub> showing decomposition of **2** (°) to (2-Ph-C<sub>6</sub>H<sub>4</sub>)BiCl<sub>2</sub> (**6**) (\*) and the formation of C<sub>6</sub>H<sub>5</sub>-C<sub>6</sub>H<sub>5</sub> (\*\*).



**Figure S2.** Time dependent <sup>1</sup>H NMR spectra of the stability of (2-Ph-C<sub>6</sub>H<sub>4</sub>)BiBr<sub>2</sub> (**7**) in CD<sub>2</sub>Cl<sub>2</sub> showing decomposition of **7** (\*) and the formation of C<sub>6</sub>H<sub>5</sub>-C<sub>6</sub>H<sub>5</sub> (\*\*).

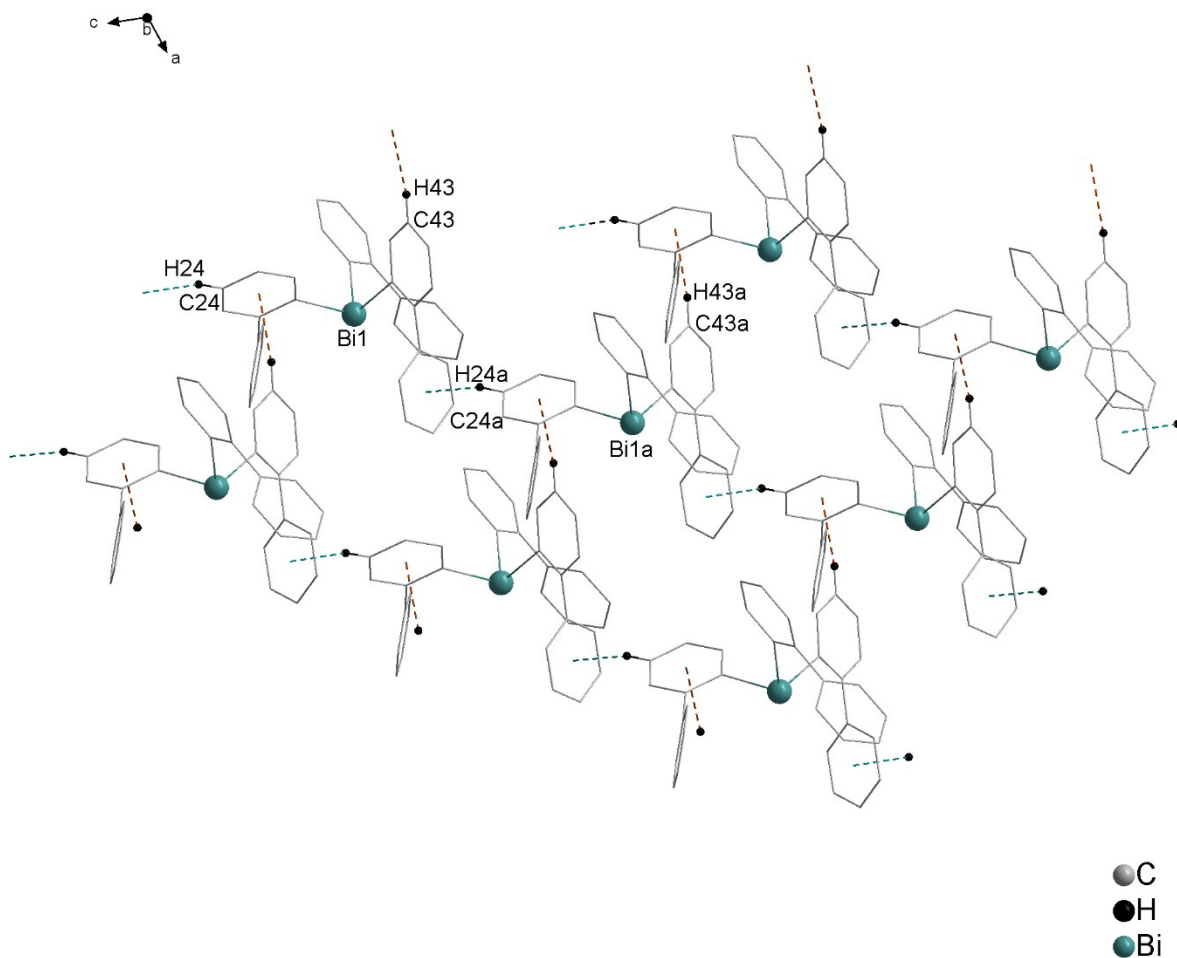


**Figure S3.** *i)* Thermal ellipsoid model of  $(2\text{-Ph-C}_6\text{H}_4)_3\text{Sb}$  (**9**) at 50% probability level. Hydrogen atoms were omitted for clarity [only hydrogen atoms involved in  $\text{C-H}\cdots\text{Ph}_{\text{centroid}}$  contacts are shown]. Selected bond lengths [Å]:  $\text{Sb1-C1}$  2.1698(16),  $\text{Sb1-C13}$  2.1608(16),  $\text{Sb1-C25}$  2.1637(16),  $\text{Sb1}\cdots\text{Ph}_{\text{centroid(I)}}$  4.05,  $\text{Sb1}\cdots\text{Ph}_{\text{centroid(II)}}$  4.05,  $\text{Sb1}\cdots\text{Ph}_{\text{centroid(III)}}$  4.00. Selected bond angles [°]:  $\text{C1-Sb1-C13}$  96.46(6),  $\text{C1-Sb1-C25}$  93.78(6),  $\text{C13-Sb1-C25}$  97.25(6),  $\text{Sb1-C1-C6}$  118.33(12),  $\text{Sb1-C13-C18}$  118.54(12),  $\text{Sb1-C25-C30}$  117.96(12). *ii)* Wire and stick model of 1D ribbon (view along the *a*-axis):  $\text{C4-H009}\cdots\text{Ph}_{\text{centroid}}$  2.504 Å (teal dashed line,  $\gamma = 4.5^\circ$ ). *iii)* wire and stick model of 2D network formed via  $\text{C15-H00K}\cdots\text{Ph}_{\text{centroid}}$  3.050 Å (violet dashed line,  $\gamma = 19.1^\circ$ ). Symmetry transformations:  $a = \frac{1}{2} + x$ ,  $\frac{3}{2} - y$ ,  $\frac{1}{2} + z$ .

#### *Solid state structure of $(2\text{-Ph-C}_6\text{H}_4)_3\text{Sb}$ (**9**)*

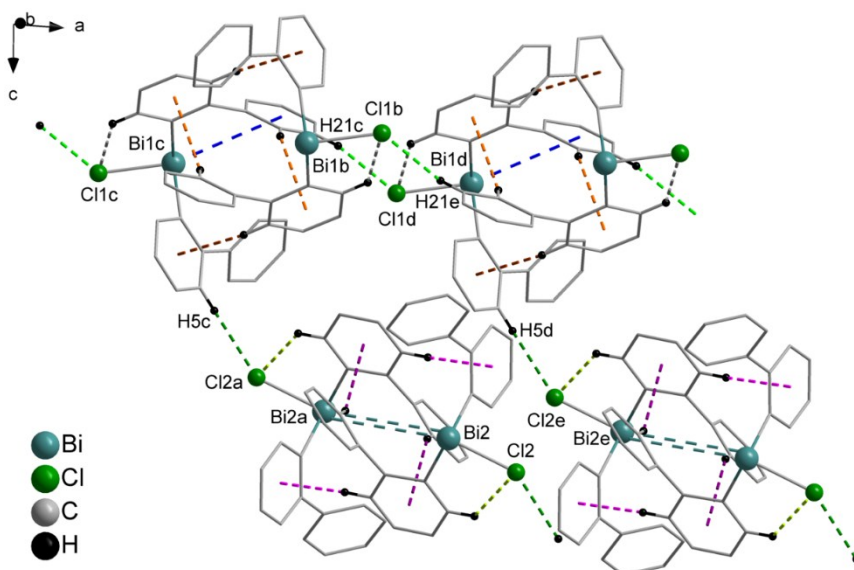
Single crystals of compound **9** suitable for X-ray diffraction were grown from a  $\text{CH}_2\text{Cl}_2$  solution at ambient temperature. The molecular structure of **9** is shown in Figure S3, the selected bond lengths and angles are listed in the Figure caption and the crystallographic data are given in

Table S2. Compound **9** crystallizes in the same monoclinic space group  $P2_1/n$  as **1** and are isostructural, showing similar molecular structures in the solid state, with a trigonal pyramidal geometry at the antimony atom. For **9** the average value of the Sb–C bond lengths of 2.165 Å is similar to those found in other antimony compounds, i.e.  $\text{Ph}_3\text{Sb}$  (2.154 Å, for an average value of C–Sb–C bond angles of  $97.2^\circ$ ),<sup>2</sup> (*p*-tolyl)<sub>3</sub>Sb (2.141 Å, for an average value of C–Sb–C bond angles of  $97.3^\circ$ ),<sup>3</sup> (*o*-tolyl)<sub>3</sub>Sb (polymorph **a**: 2.166 Å; polymorph **b**: 2.162 Å; average value of C–Sb–C bond angles of  $97.4^\circ$ , and  $96.7^\circ$ , respectively),<sup>4</sup> but significantly smaller than those found in the polymorphs of  $\text{Me}_3\text{Sb}$  (polymorph **a**: 2.184 Å; polymorph **b**: 2.182 Å; ; average value of C–Sb–C bond angles of  $105.6^\circ$ , and  $105.0^\circ$ , respectively).<sup>5</sup> The dispersion type  $\text{Sb}\cdots\text{Ph}_{\text{centroid}}$  interaction of av. 4.04 Å in **9** are not distinct from those as observed for the analogous bismuth compound **1**. However, the presence of  $\text{C–H}\cdots\text{Ph}_{\text{centroid}}$  contacts dominates also in the structure of **9**, which forms 1D ribbon via  $\text{C–H}\cdots\text{Ph}_{\text{centroid}}$  intermolecular contacts with  $\text{C4–H009}\cdots\text{Ph}_{\text{centroid}}$  2.50 Å (teal dashed line,  $\gamma = 4.5^\circ$ ). Furthermore, the 1D ribbon are connected via additional intermolecular contacts with  $\text{C15–H00K}\cdots\text{Ph}_{\text{centroid}}$  3.05 Å to give a 2D network.

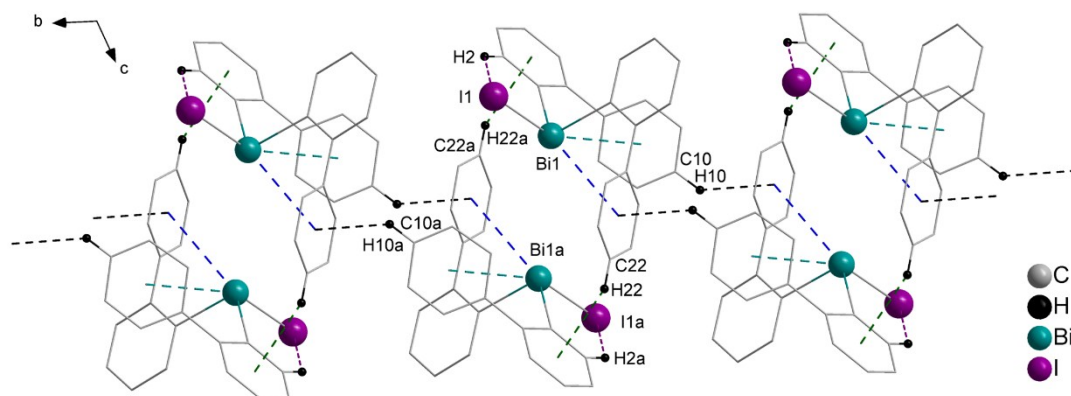


**Figure S4.** Wire and stick model of  $(2\text{-PhC}_6\text{H}_4)_3\text{Bi}$  (**1**). Hydrogen atoms were omitted for clarity [only hydrogen atoms involved in  $\text{C-H}\cdots\text{Ph}_{\text{centroid}}$  contacts are shown]. *i*) 1D ribbon (view along the *a*-axis):  $\text{C24-H24}\cdots\text{Ph}_{\text{centroid}}$  2.55 Å (teal dashed line,  $\gamma = 5.6^\circ$ ). *ii*) wire and stick model of 2D network (view along the *b*-axis) formed via  $\text{C43-H43}\cdots\text{Ph}_{\text{centroid}}$  3.06 (violet dashed line,  $\gamma = 10.3^\circ$ ). Symmetry transformations:  $a = \frac{1}{2} + x$ ,  $\frac{1}{2} - y$ ,  $-\frac{1}{2} + z$ .

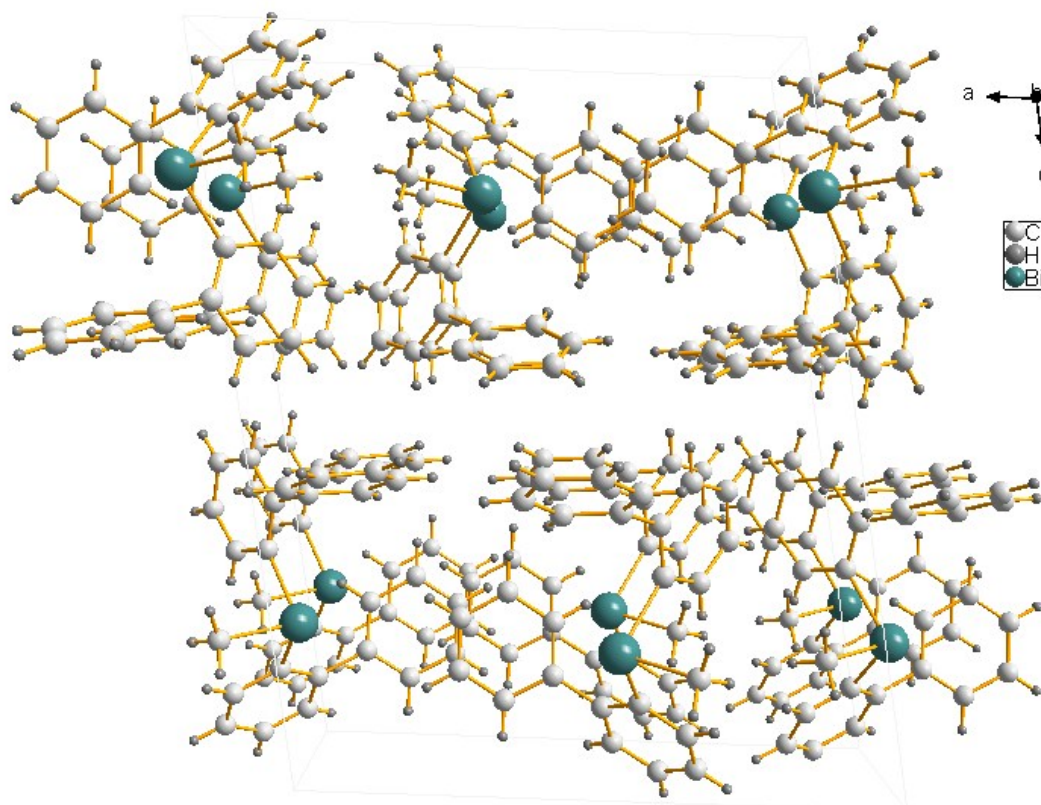




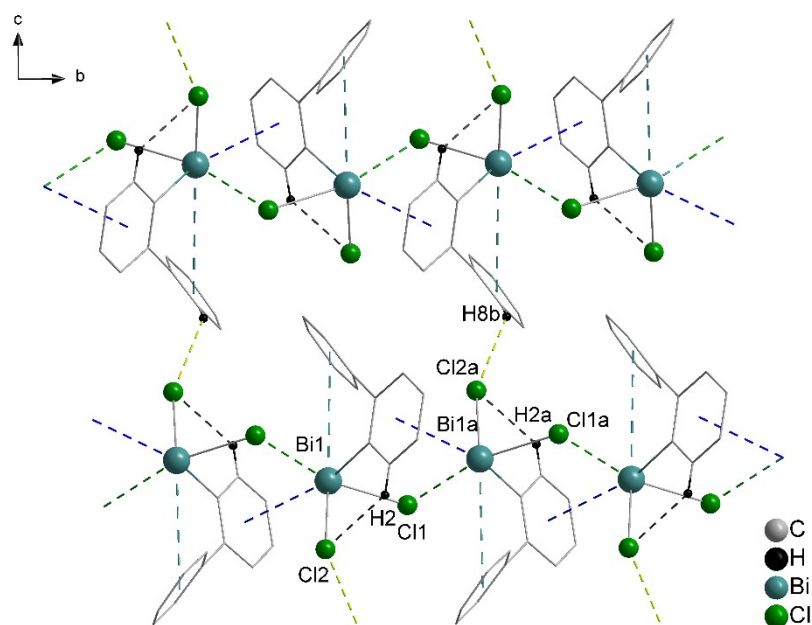
**Figure S5.** Wire and stick model of 2D network (view along the *b*-axis) of  $(2\text{-PhC}_6\text{H}_4)_2\text{BiCl}$  (**2**) formed via Cl $\cdots$ H intermolecular contacts: C5c–H5c $\cdots$ Cl2a 2.75 Å (bright green dashed line), C21e–H21e $\cdots$ Cl1b 2.86 Å (green dashed line). Symmetry transformations:  $a = 1 - x, -y, 1 - z$ ,  $b = -x, 1 - y, -z$ ;  $c = x, -1 + y, z$ ;  $d = 1 + x, 1 + y, z$ ;  $e = 1 - x, 1 - y, -z$ .



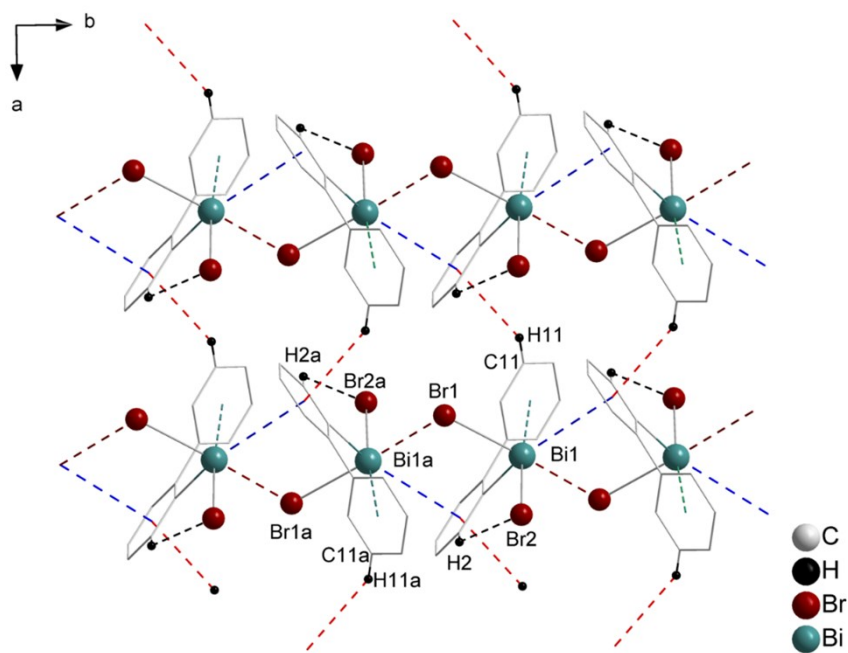
**Figure S6.** Wire and stick model of 1D ribbon (view along the *a*-axis) of  $(2\text{-PhC}_6\text{H}_4)_2\text{BiI}$  (**4**) formed via intermolecular contacts C10–H10 $\cdots$ Ph<sub>centroid</sub> 2.81 Å (black dashed line,  $\gamma = 10.7^\circ$ ). Symmetry transformations:  $a = 1 - x, 1 - y, 1 - z$ .



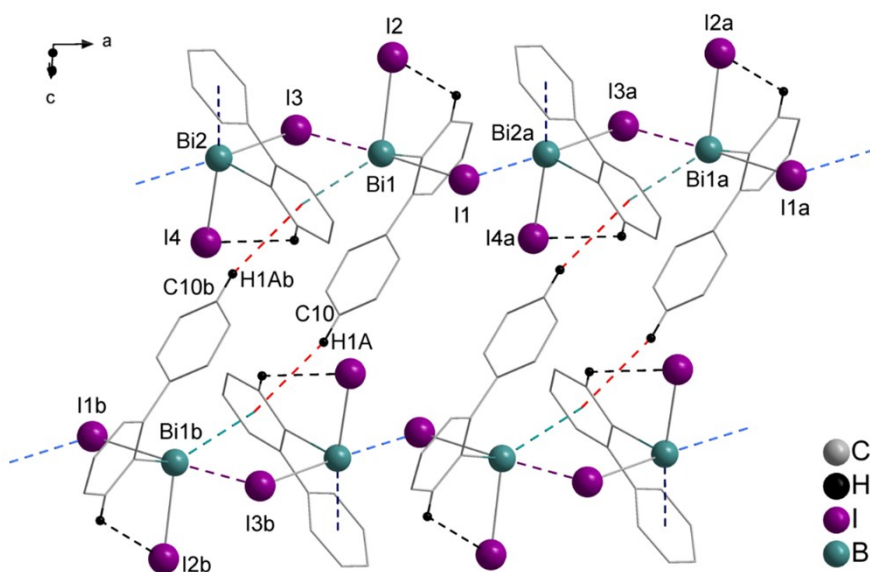
**Figure S7.** Ball and stick model of  $(2\text{-Ph-C}_6\text{H}_4)_2\text{BiMe}$  (**5**); view along *b* axis.



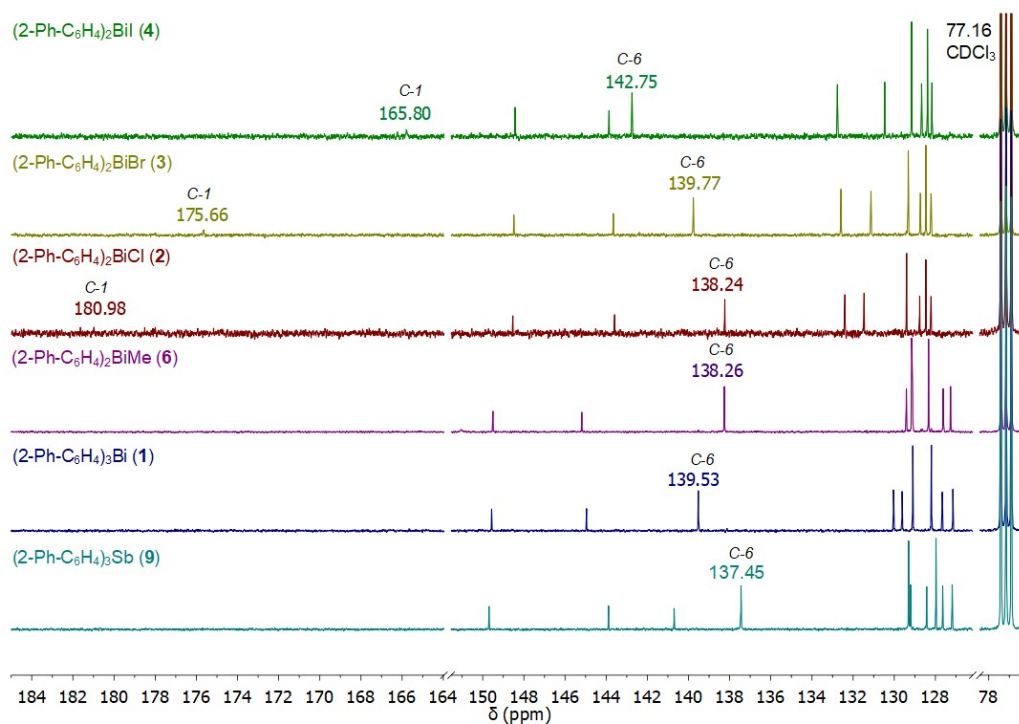
**Figure S8.** Wire and stick model of 2D network (view along the *a*-axis) of  $(2\text{-PhC}_6\text{H}_4)\text{BiCl}_2$  (**6**) formed via  $\text{H}\cdots\text{Cl}$  intermolecular contacts  $\text{C8b-H8b}\cdots\text{Cl2a}$  2.81 Å (lime dashed line). Symmetry transformations:  $a = 2 - x, \frac{1}{2} + y, \frac{1}{2} - z$ ,  $b = -\frac{1}{2} + x, \frac{3}{2} - y, 1 - z$ .



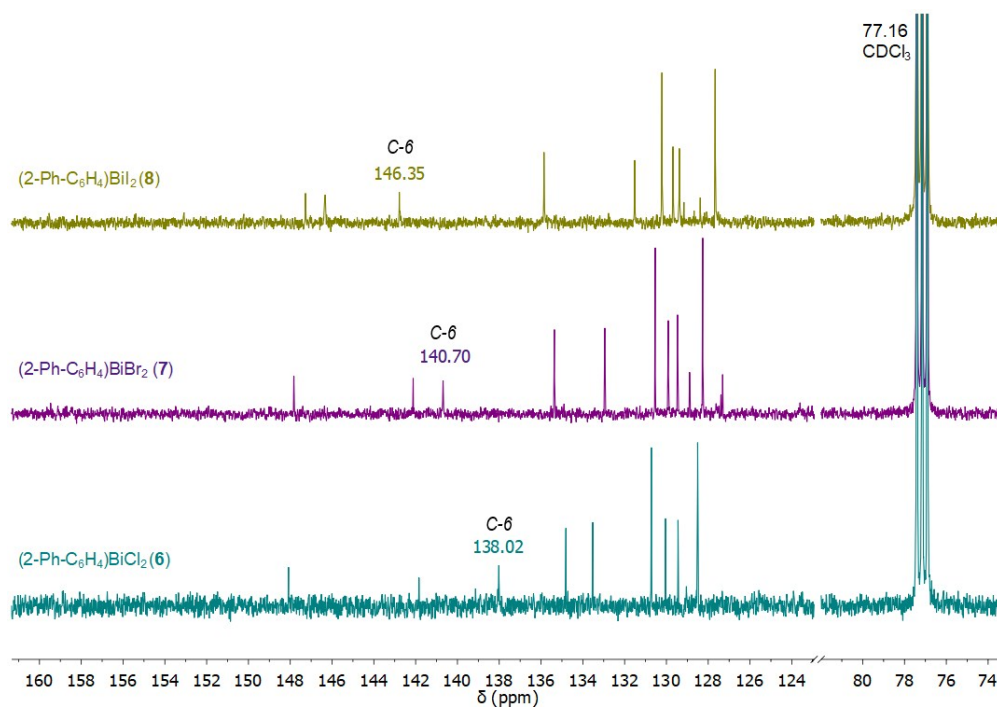
**Figure S9.** Wire and stick model of 2D network (view along the *c*-axis) of (2-PhC<sub>6</sub>H<sub>4</sub>)BiBr<sub>2</sub> (**7**) formed via intermolecular contacts C11–H11⋯Ph<sub>centroid</sub> 2.84 Å (red dashed line,  $\gamma = 13.1^\circ$ ). Symmetry transformations:  $a = -x, \frac{1}{2} + y, \frac{1}{2} - z$ .



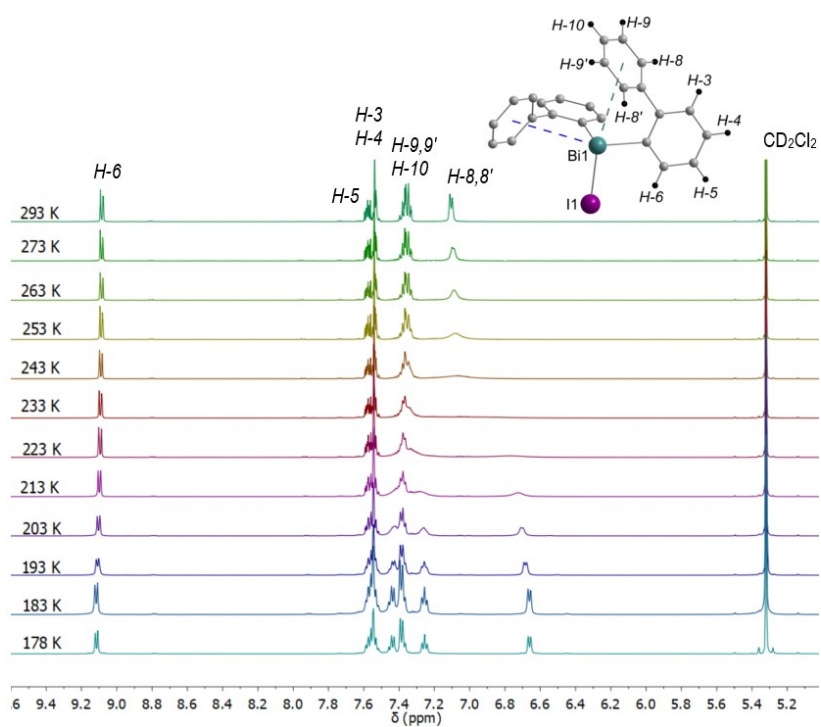
**Figure S10.** Wire and stick model of 2D network (view along the *b*-axis) of (2-PhC<sub>6</sub>H<sub>4</sub>)BiI<sub>2</sub> (**8**) formed via intermolecular contacts C10–H1A⋯Ph<sub>centroid</sub> 2.87 Å (red dashed line,  $\gamma = 17.1^\circ$ ). Symmetry transformations:  $a = 1 + x, y, z, b = -x, 1 - y, 1 - z$ .



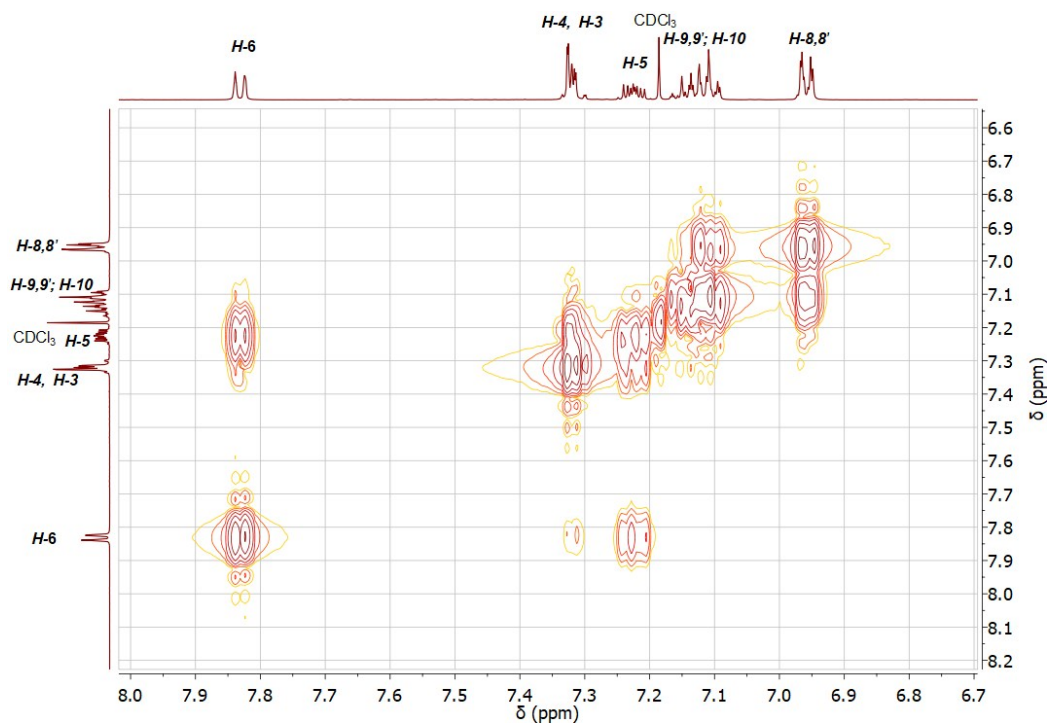
**Figure S11.** Comparison of  $^{13}\text{C}$  NMR spectra (aromatic region) in  $\text{CDCl}_3$  of compounds 1–5 and 9 showing a large downfield shifts for the resonances belonging to C-6 placed in *ortho* position to bismuth atom and for C-1 of compounds 2–4, respectively.



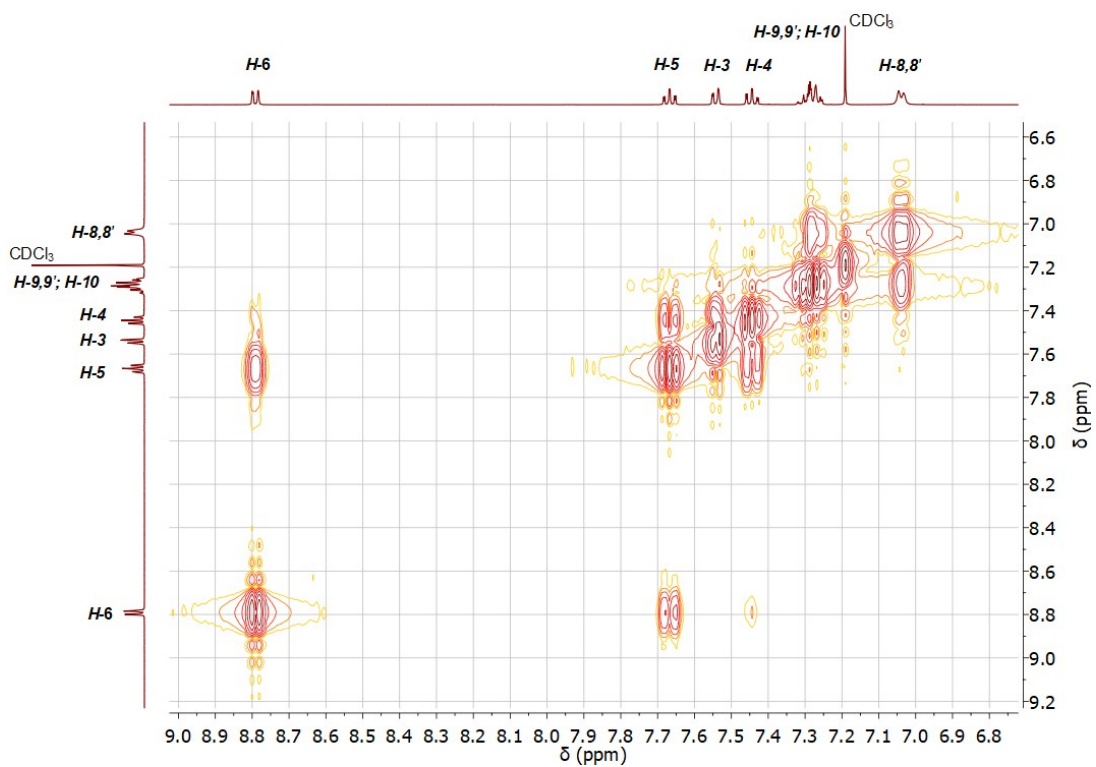
**Figure S12.** Comparison of  $^{13}\text{C}$  NMR spectra (aromatic region) in  $\text{CDCl}_3$  of compounds 6–8 showing a large downfield shifts for the resonances belonging to C-6 placed in *ortho* position to bismuth atom.



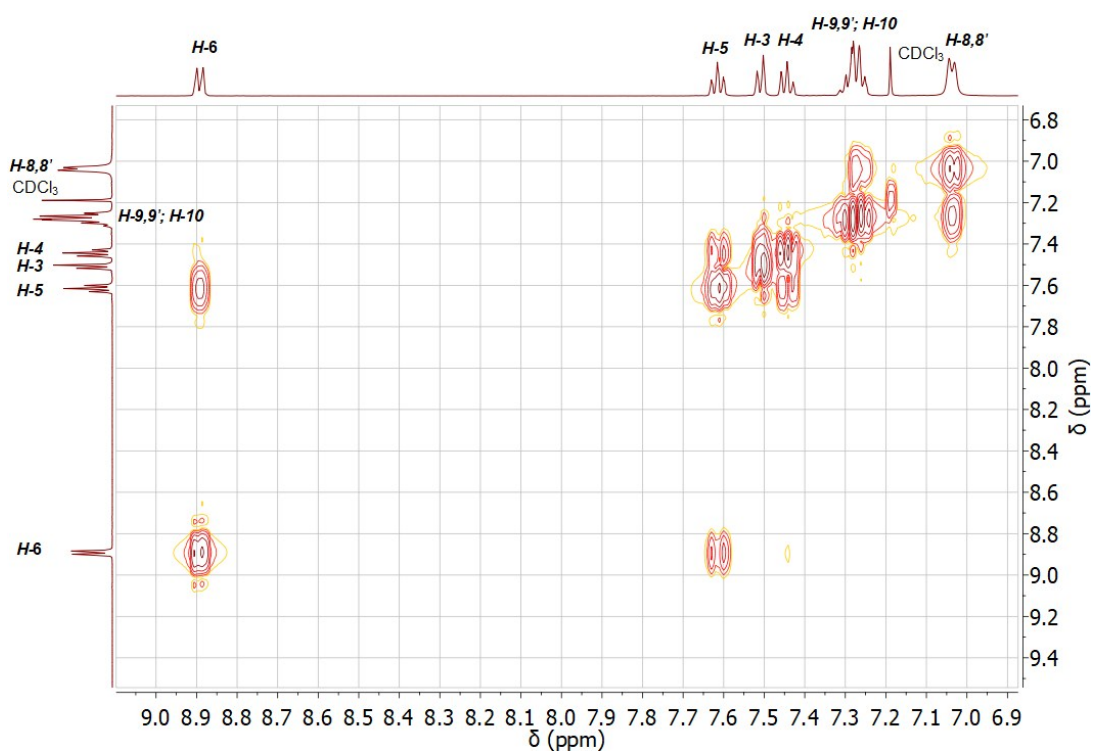
**Figure S13.** Temperature dependent  $^1\text{H}$  NMR spectra of  $(2\text{-PhC}_6\text{H}_4)_2\text{Bil}$  (**4**) measured in  $\text{CD}_2\text{Cl}_2$ , showing the region for aromatic protons including the numbering scheme.



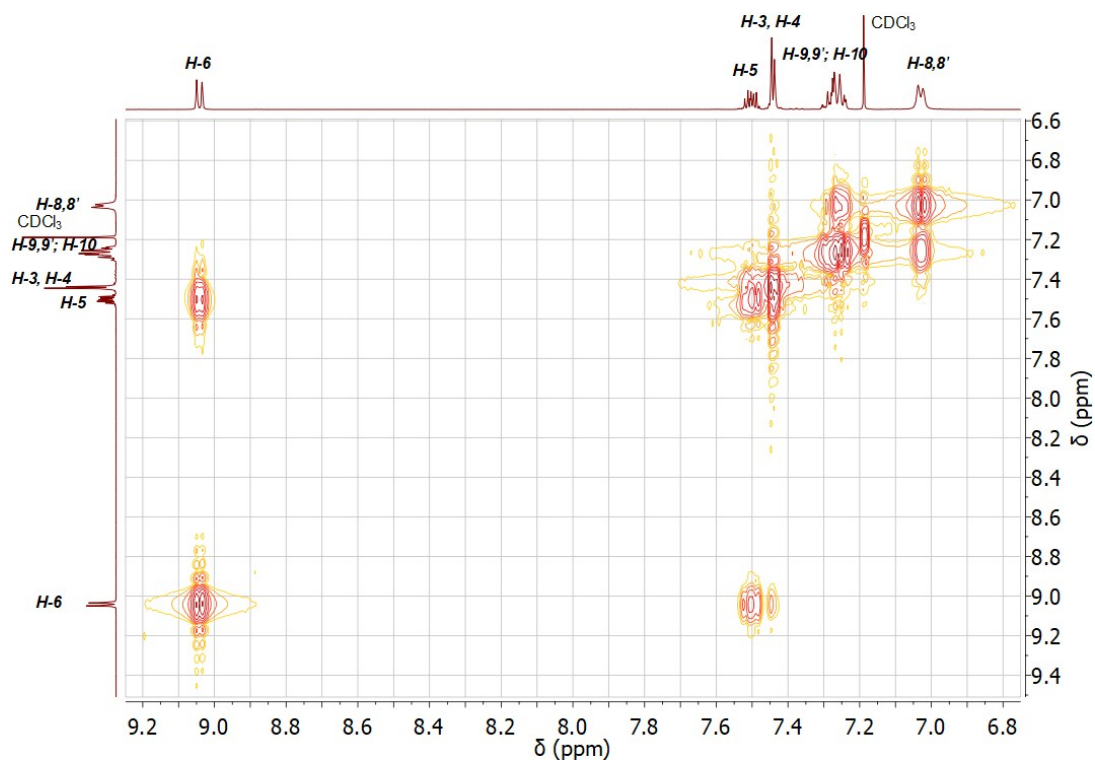
**Figure S14.**  $^1\text{H}$ - $^1\text{H}$  COSY NMR spectrum of  $(2\text{-Ph-C}_6\text{H}_4)_3\text{Bi}$  (**1**) in  $\text{CDCl}_3$  at 500.30 MHz.



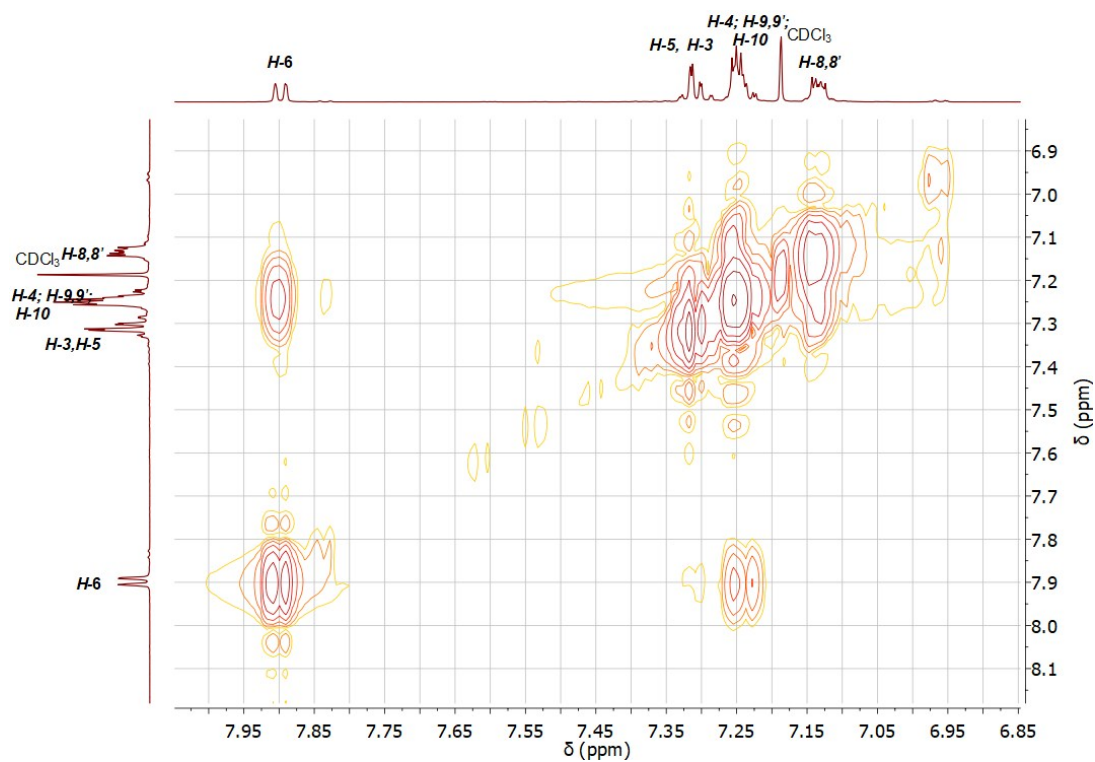
**Figure S15.**  $^1\text{H}$ - $^1\text{H}$  COSY NMR spectrum of  $(2\text{-Ph-C}_6\text{H}_4)_2\text{BiCl}$  (**2**) in  $\text{CDCl}_3$  at 500.30 MHz.



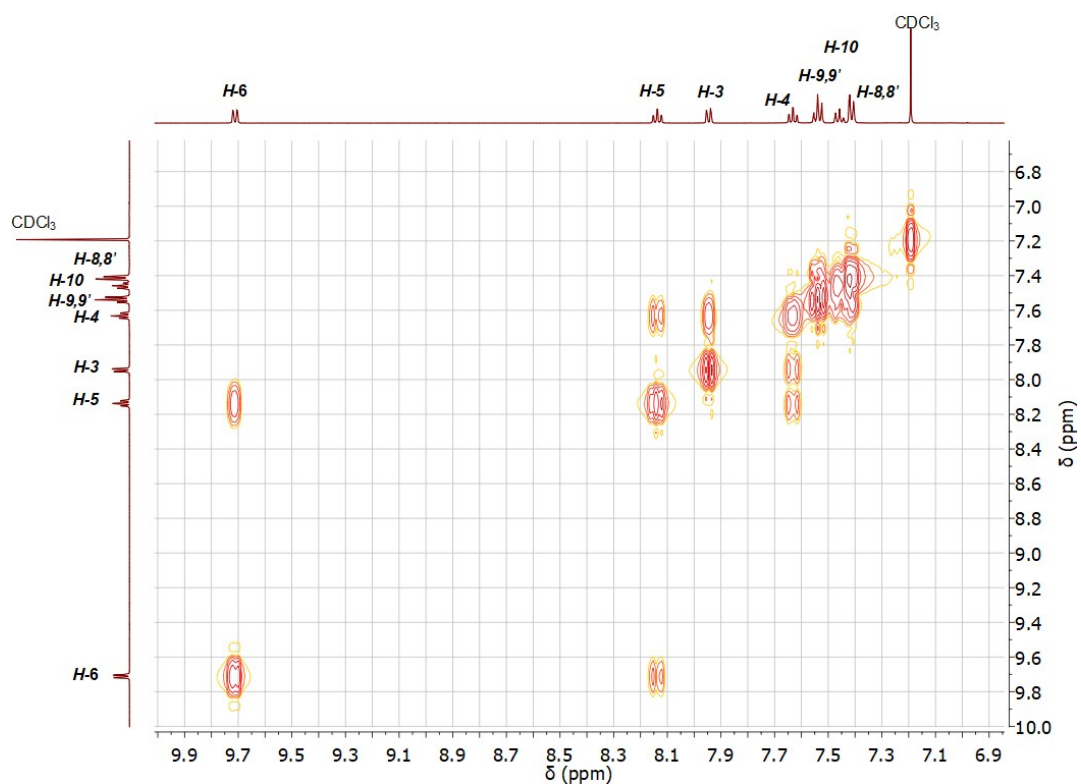
**Figure S16.**  $^1\text{H}$ - $^1\text{H}$  COSY NMR spectrum of  $(2\text{-Ph-C}_6\text{H}_4)_2\text{BiBr}$  (**3**) in  $\text{CDCl}_3$  at 500.30 MHz.



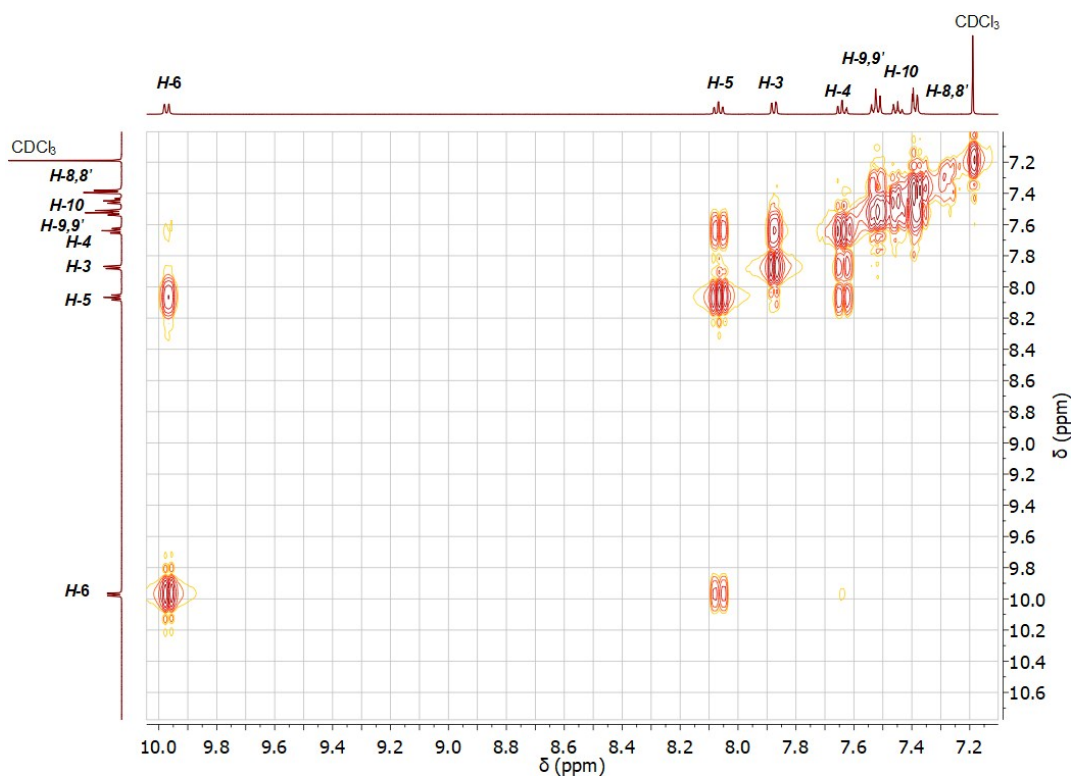
**Figure S17.**  $^1\text{H}$ - $^1\text{H}$  COSY NMR spectrum of (2-Ph- $\text{C}_6\text{H}_4$ ) $_2$ BiI (**4**) in  $\text{CDCl}_3$  at 500.30 MHz.



**Figure S18.**  $^1\text{H}$ - $^1\text{H}$  COSY NMR spectrum of (2-Ph- $\text{C}_6\text{H}_4$ ) $_2$ BiMe (**5**) in  $\text{CDCl}_3$  at 500.30 MHz.

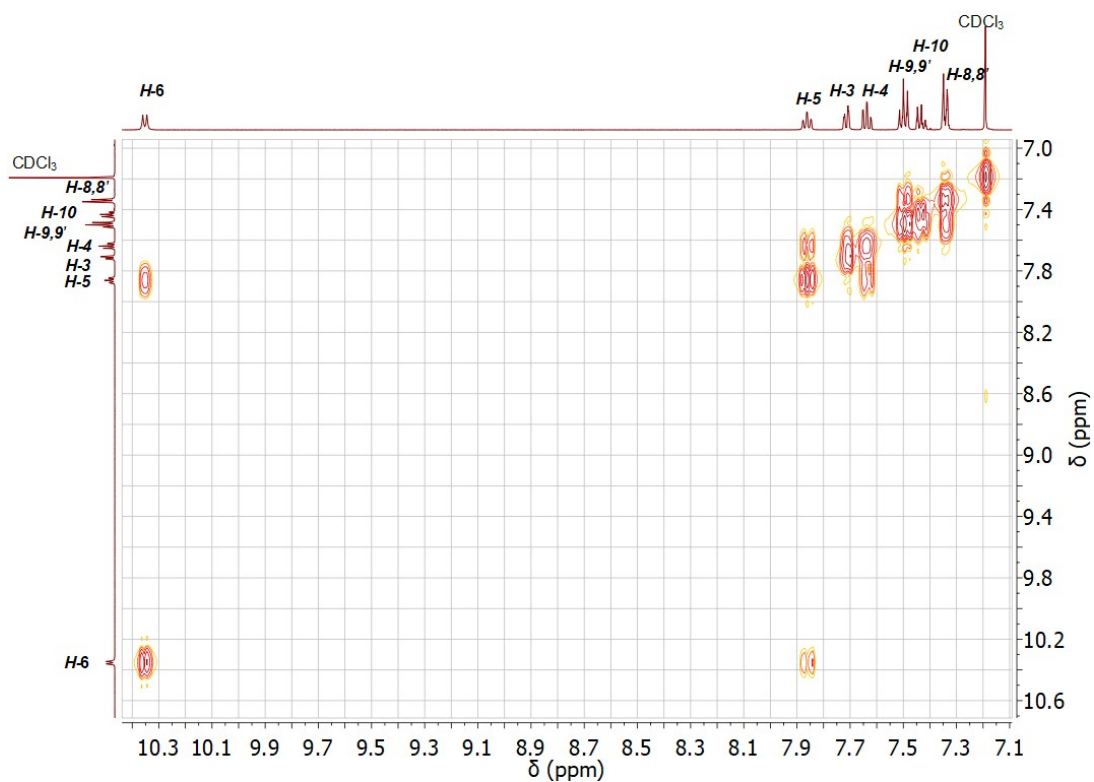


**Figure S19.** <sup>1</sup>H-<sup>1</sup>H COSY NMR spectrum of (2-Ph-C<sub>6</sub>H<sub>4</sub>)BiCl<sub>2</sub> (**6**) in CDCl<sub>3</sub> at 500.30 MHz.

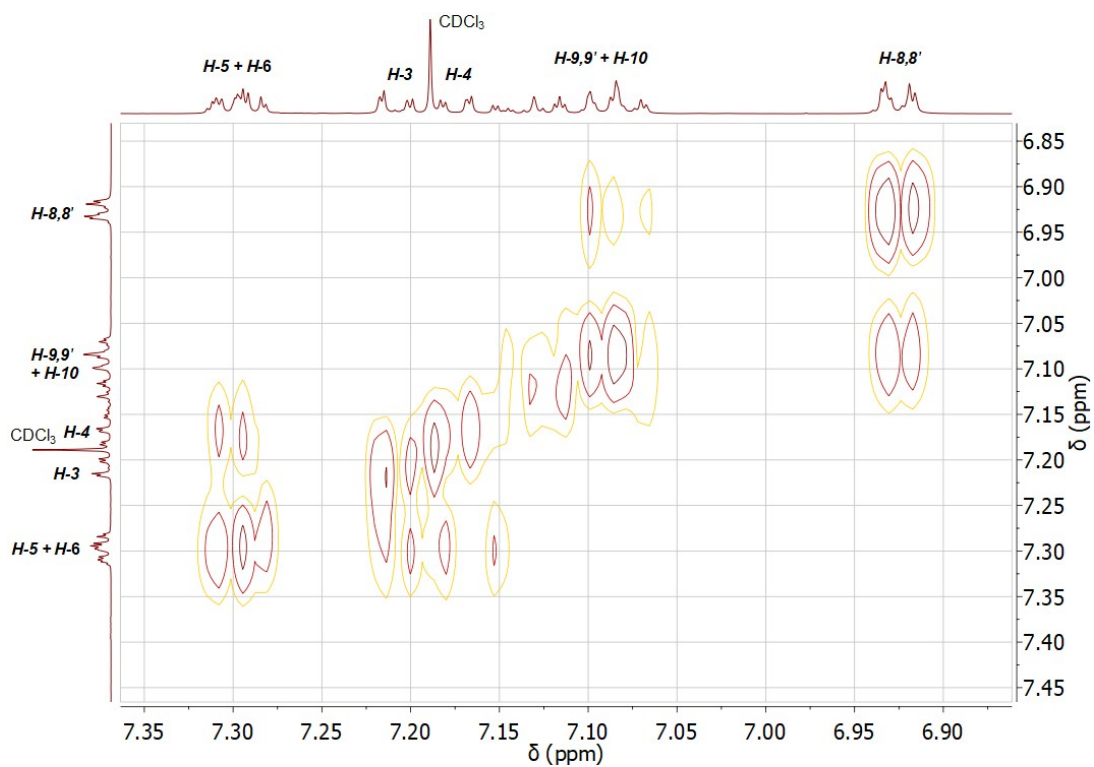


**Figure S20.** <sup>1</sup>H-<sup>1</sup>H COSY NMR spectrum of (2-Ph-C<sub>6</sub>H<sub>4</sub>)BiBr<sub>2</sub> (**7**) in CDCl<sub>3</sub> at 500.30 MHz.

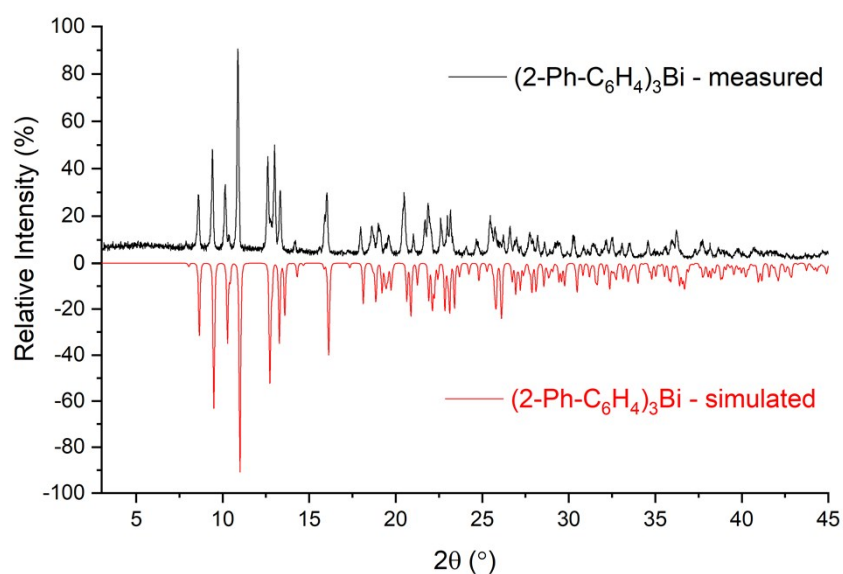




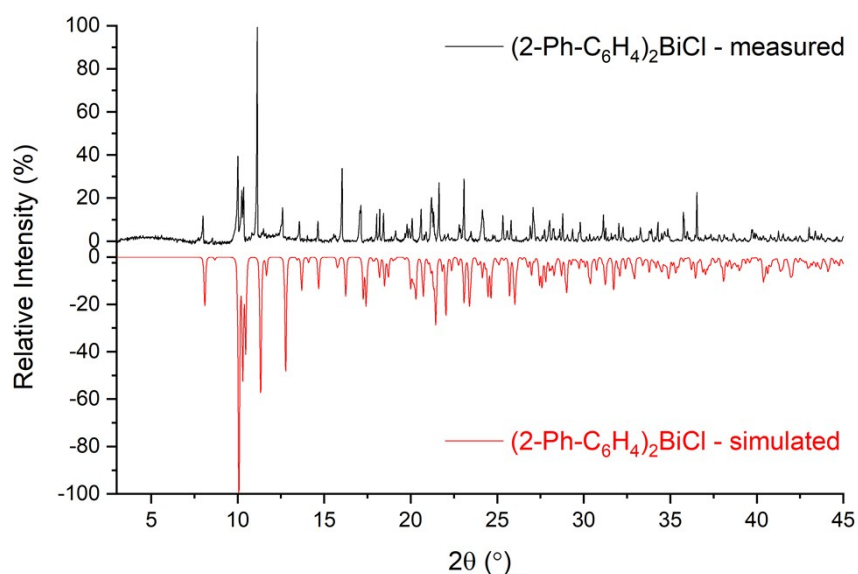
**Figure S21.**  $^1\text{H}$ - $^1\text{H}$  COSY NMR spectrum of  $(2\text{-Ph-C}_6\text{H}_4)\text{Bi}_2$  (**8**) in  $\text{CDCl}_3$  at 500.30 MHz.



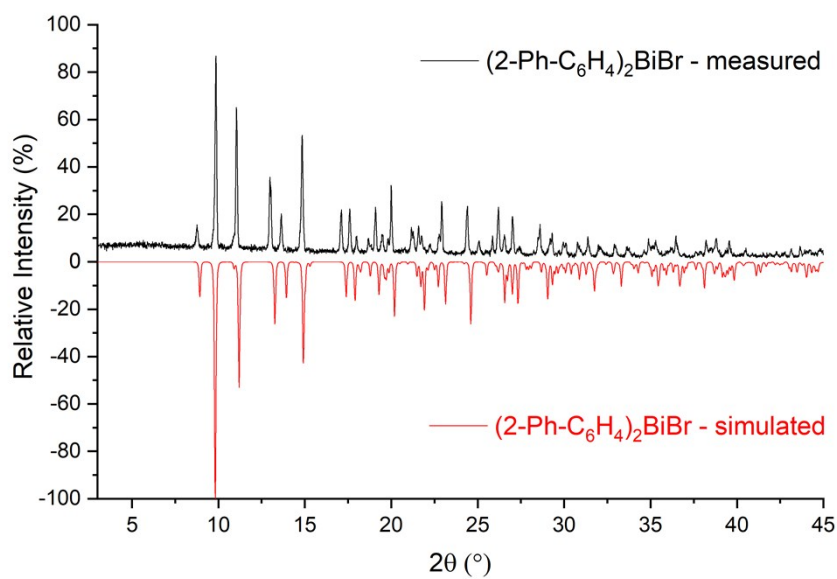
**Figure S22.**  $^1\text{H}$ - $^1\text{H}$  COSY NMR spectrum of  $(2\text{-Ph-C}_6\text{H}_4)_3\text{Sb}$  (**9**) in  $\text{CDCl}_3$  at 500.30 MHz.



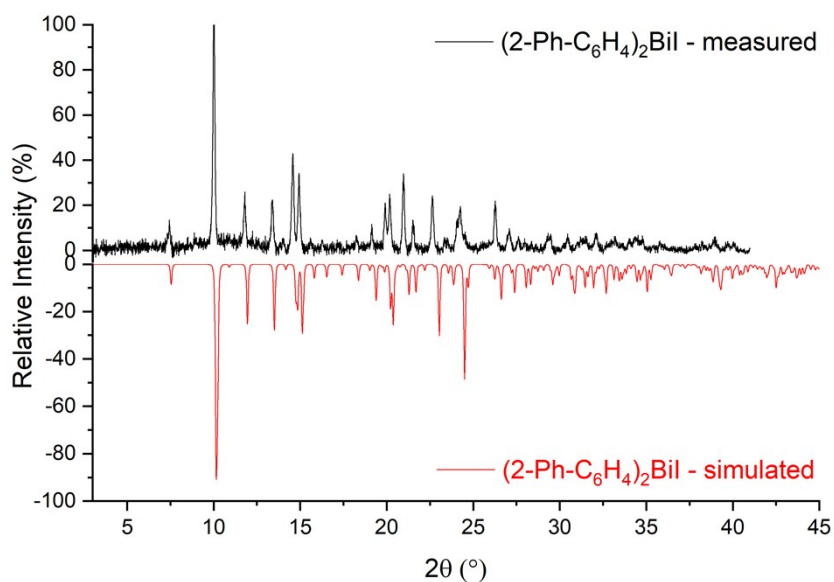
**Figure S23.** Powder X-ray diffraction pattern of  $(2\text{-Ph-C}_6\text{H}_4)_3\text{Bi}$  (**1**) at 293 K, measured for isolated material (black) and calculated from single crystal X-ray data measured at 120 K (red).



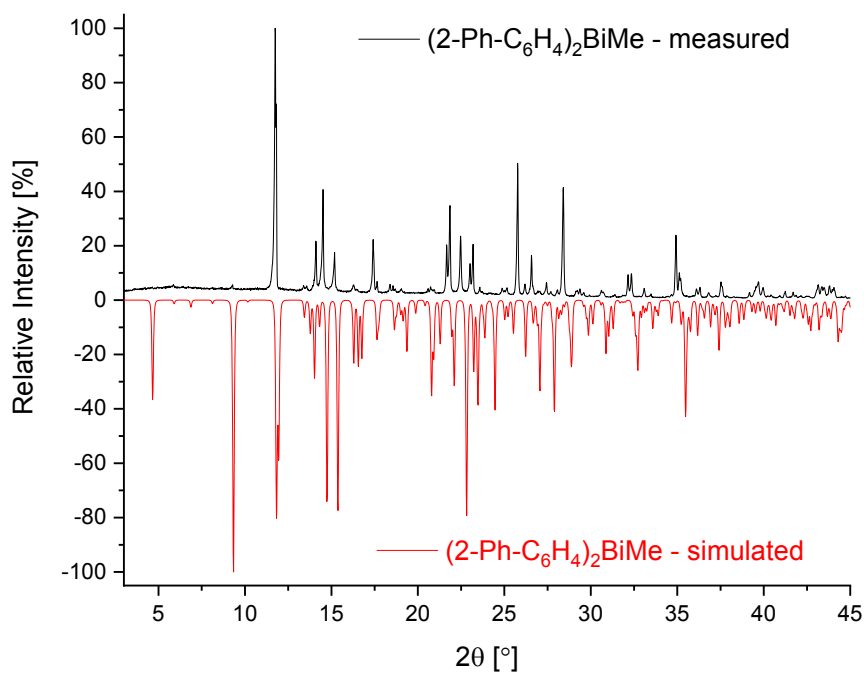
**Figure S24.** Powder X-ray diffraction pattern of  $(2\text{-Ph-C}_6\text{H}_4)_2\text{BiCl}$  (**2**) at 293 K, measured for isolated material (black) and calculated from single crystal X-ray data measured at 100 K (red).



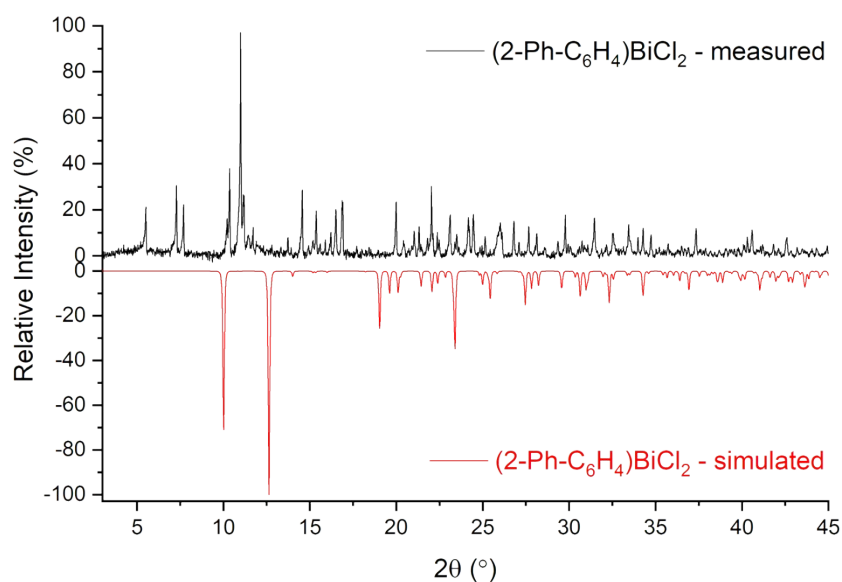
**Figure S25.** Powder X-ray diffraction pattern of  $(2\text{-Ph-C}_6\text{H}_4)_2\text{BiBr}$  (**3**) at 293 K, measured for isolated material (black) and calculated from single crystal X-ray data measured at 115.7 K (red).



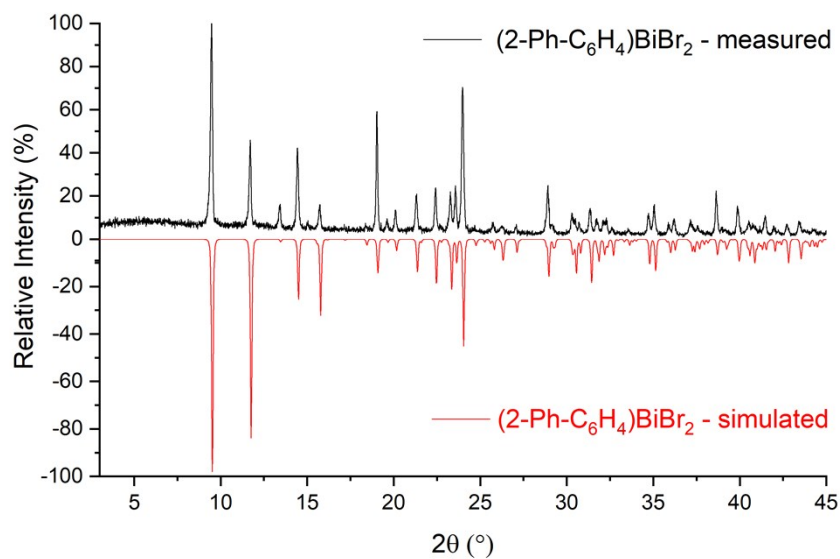
**Figure S26.** Powder X-ray diffraction pattern of  $(2\text{-Ph-C}_6\text{H}_4)_2\text{BiI}$  (**4**) at 293 K, measured for isolated material (black) and calculated from single crystal X-ray data measured at 100 K (red).



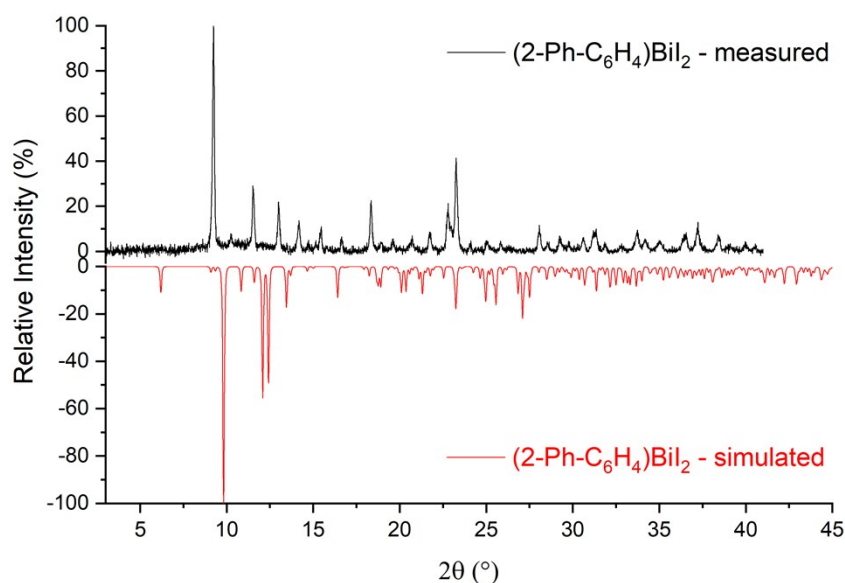
**Figure S27.** Powder X-ray diffraction pattern of  $(2\text{-Ph-C}_6\text{H}_4)_2\text{BiMe}$  (**5**) at 293 K, measured for isolated needles (black) and calculated from single crystal X-ray data measured at 100 K (red). We attribute the difference of the diffractograms to the formation of different polymorphs at ambient and low temperature.



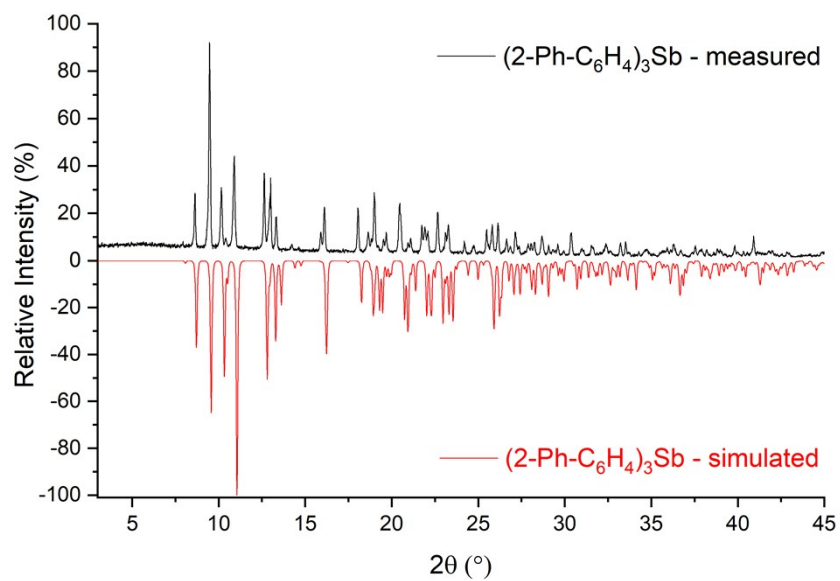
**Figure S28.** Powder X-ray diffraction pattern of  $(2\text{-Ph-C}_6\text{H}_4)\text{BiCl}_2$  (**6**) at 293 K, measured for isolated material (black) and calculated from single crystal X-ray data measured at 100 K (red). We attribute the difference of the diffractograms to the formation of different polymorphs at ambient and low temperature.



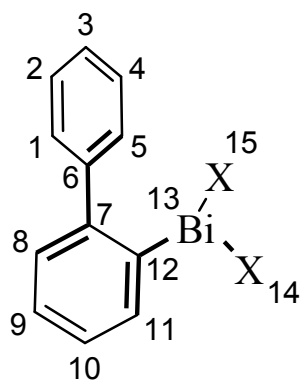
**Figure S29.** Powder X-ray diffraction pattern of  $(2\text{-Ph-C}_6\text{H}_4)\text{BiBr}_2$  (**7**) at 293 K, measured for isolated material (black) and calculated from single crystal X-ray data measured at 293 K (red).



**Figure S30.** Powder X-ray diffraction pattern of  $(2\text{-Ph-C}_6\text{H}_4)\text{BiI}_2$  (**8**) at 293 K, measured for isolated material (black) and calculated from single crystal X-ray data measured at 100 K (red). We attribute the difference of the diffractograms to the formation of different polymorphs at ambient and low temperature.



**Figure S31.** Powder X-ray diffraction pattern of (2-Ph-C<sub>6</sub>H<sub>4</sub>)<sub>3</sub>Sb (**9**) at 293 K, measured for isolated material (black) and calculated from single crystal X-ray data measured at 100 K (red).



**Figure S32.** Definition of the dihedral angle  $\alpha$  and  $\beta$  displayed in Fig. 17 and 18 in the main manuscript: **C11-C12-Bi13-X14** and **C8-C7-C6-C5**, respectively (in bold). These angle notations have been used to perform the relaxed dihedral angle scan which are described in main manuscript. Hydrogen atoms have been omitted for clarity.

**RBiCl<sub>2</sub>** (R =2-PhC<sub>6</sub>H<sub>4</sub>)

Coordinates of structure 1:

C	0.120020090	1.247940601	0.066203983
C	0.262380137	2.029158668	-1.098691705
C	1.180857834	3.083771341	-1.148595617
C	1.958176773	3.381142116	-0.029812365
C	1.802690526	2.631981855	1.140890100
C	0.893494471	1.576885567	1.189671744
C	-0.773952488	0.065657604	0.063051402
C	-0.589279619	-0.924281620	-0.921997382
C	-1.415802292	-2.049240581	-0.945989259
C	-2.419267897	-2.201855692	0.015251930
C	-2.590024056	-1.233317815	1.007365537
C	-1.767753475	-0.106260013	1.036985370
H	-0.410627226	1.851623385	-1.942572610
H	1.271950565	3.682669568	-2.055442247
H	2.678220371	4.198934867	-0.064967428
H	2.409257472	2.861683667	2.017381301
H	0.802287012	0.969726367	2.090584202
H	-1.259589734	-2.823270039	-1.700178690
H	-3.061560405	-3.083480656	-0.004611877
H	-3.369290922	-1.354524703	1.761064951
H	-1.906413143	0.656365877	1.805942815
Bi	1.155635922	-0.629936842	-2.343316680
Cl	0.830311963	-2.841416797	-3.455833973
Cl	2.879555430	-1.187529816	-0.647679742



Coordinates of structure 2:

C	0.161940613091	1.275778410348	0.092631867519
C	0.383080537943	1.954401280542	-1.123437668849
C	1.225386466170	3.068449409429	-1.182488065279
C	1.850535719513	3.530466634708	-0.023992317830
C	1.621815469055	2.879604244469	1.192365415271
C	0.786871176633	1.764049267795	1.251316861623
C	-0.681307379409	0.057138373429	0.116538826552
C	-0.420716124932	-0.981778189740	-0.796352515607
C	-1.228317782939	-2.121596841110	-0.809807207272
C	-2.286071042597	-2.241285151594	0.093549240018
C	-2.531952550184	-1.223377104710	1.020218052052
C	-1.733281813454	-0.080830452106	1.036356595131
H	-0.173090665375	1.641692389872	-2.012131215314
H	1.374965651343	3.585482490543	-2.130703647468
H	2.506211275425	4.400312733194	-0.064941206990
H	2.107362954912	3.238169309225	2.100337095893
H	0.629739334555	1.244337566976	2.197054900740
H	-1.022131546954	-2.927890001937	-1.516464887136
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H	-1.938438920131	0.724016545659	1.744851815124
Bi	1.449594355658	-0.824359166797	-2.060455271621
Cl	0.389599049650	-1.860572186405	-4.054021828148
Cl	2.480582265655	-2.849707828005	-1.044962424014

Coordinates of structure 3:

C	0.151070544897	1.261666858010	0.090174123225
C	0.496764252184	1.817865767682	-1.158599377894
C	1.341567598077	2.929976496469	-1.237762008916
C	1.837759071291	3.515059245468	-0.073138261391
C	1.479185291723	2.988054944246	1.171782386320
C	0.645638137414	1.873193917269	1.253945166226
C	-0.672042270243	0.030880075137	0.154287264724
C	-0.312627642387	-1.088585164611	-0.622919431878
C	-1.076746740929	-2.256142182572	-0.563115531622
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C	-2.551042393976	-1.216850595820	1.049255234825
C	-1.788399379873	-0.050553009661	1.001870274265
H	0.041582542275	1.419015372230	-2.069934247343
H	1.591365706495	3.347322458277	-2.213422979127
H	2.493560041503	4.383876674535	-0.131799274932
H	1.861271629869	3.443658743932	2.085723903039
H	0.390256124395	1.449627747020	2.225986928420
H	-0.782352621420	-3.127939725579	-1.150122874114
H	-2.795316002091	-3.231992639290	0.305642603583
H	-3.426854064852	-1.264698207686	1.697420557192
H	-2.069976660616	0.815126201040	1.603839592231
Bi	1.608361626216	-0.947491148312	-1.814832270257
Cl	0.548955629201	-0.551128892326	-4.030996011423
Cl	1.868137805737	-3.417931138152	-2.004471368953

Coordinates of structure 4:

C	0.144230168215	1.187584677600	-0.107335903959
C	-0.274010319909	2.195700276862	-0.990527198553
C	0.451837274752	3.380454084482	-1.108683949486
C	1.598126060490	3.581426962544	-0.335607663226
C	2.017111115096	2.588905785517	0.551700281436
C	1.297148930625	1.399658112625	0.661248504429
C	-0.651499167549	-0.051674948107	0.054994999083
C	-0.107638480000	-1.341421607145	-0.091479928205
C	-0.912051278830	-2.462901691407	0.160908772193
C	-2.251775468951	-2.334728546561	0.530461999342
C	-2.801407849139	-1.057495618099	0.638614282113
C	-2.008272236998	0.065250463844	0.405451382290
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H	2.164412820995	4.508825115058	-0.426431165582
H	2.911609470070	2.736505956036	1.157266416202
H	1.618929837741	0.627693342275	1.361938653278
H	-0.507997782115	-3.477967095664	0.041719041803
H	-2.858999251379	-3.220054368406	0.719451922205
H	-3.848147501968	-0.932150240246	0.917135719403
H	-2.433625654715	1.063915601339	0.517900617672
Bi	1.839370720818	-2.162554377867	-0.906207902526
Cl	3.371112764757	-0.267824225624	-1.298347003620
Cl	0.962601157555	-2.407745883025	-3.209238548042

Coordinates of structure 5:

C	0.057331811089	1.164560262684	-0.225525953535
C	-0.501164795580	2.232598711226	-0.946174637722
C	0.233863505229	3.394724782600	-1.173974552681
C	1.532863741019	3.512763161899	-0.673173852091
C	2.091353272392	2.461549758527	0.055970513371
C	1.359772880292	1.296057840167	0.278327394997
C	-0.721096154860	-0.068906538042	0.021163054904
C	-0.193470502203	-1.357434943103	-0.200681897651
C	-0.964536273058	-2.487438013447	0.107631203306
C	-2.259131069785	-2.370314948107	0.618208495771
C	-2.793869658129	-1.096679864758	0.811495126661
C	-2.033850403892	0.034368958535	0.514802088897
H	-1.507509145441	2.134393067679	-1.355375529476
H	-0.205375442613	4.209144360948	-1.751391902638
H	2.108376754011	4.421323738366	-0.853639804993
H	3.103132705803	2.544312263435	0.452533388748
H	1.796007469108	0.481696926074	0.857435783638
H	-0.568108436332	-3.496756019060	-0.066953348655
H	-2.841330112533	-3.260633944744	0.856125375091
H	-3.803882492917	-0.980742877771	1.205329983506
H	-2.447456205005	1.027830253768	0.694478640723
Bi	1.682568643338	-2.065786184675	-1.235345386947
Cl	3.358607064374	-1.751523918903	0.578137481603
Cl	2.198180155691	-0.176679923297	-2.734697904828

Coordinates of structure 6:

C	0.033111805721	1.222226900289	-0.300162533469
C	-0.555534798705	2.269482502985	-1.027638257869
C	0.132206087501	3.464728895989	-1.232176174611
C	1.411646416483	3.636711826278	-0.697794412768
C	2.001387631390	2.604957312349	0.033941066112
C	1.320085131328	1.403845349294	0.226580129065
C	-0.708399846971	-0.031137227461	-0.031638368915
C	-0.157260728684	-1.308160207892	-0.254844412786
C	-0.881745449153	-2.448920376709	0.127559271145
C	-2.147860975035	-2.349854523577	0.706191929890
C	-2.709578149475	-1.086347942566	0.893897270164
C	-1.995435277102	0.053923804148	0.530789719418
H	-1.553277542093	2.134077435686	-1.447630107837
H	-0.330349899615	4.264449578777	-1.811883725045
H	1.948694666142	4.572758926981	-0.854577537525
H	3.000780235923	2.729932291888	0.450283610997
H	1.778489599969	0.598341346256	0.801824496412
H	-0.460702352832	-3.450774990043	-0.025412172051
H	-2.687355570357	-3.248437293036	1.005747143698
H	-3.699609516462	-0.986125638747	1.339237927365
H	-2.420019990842	1.042175407458	0.713732543118
Bi	1.553478577806	-2.053745571173	-1.539371934169
Cl	2.802926438654	-3.095822658108	0.334240745112
Cl	3.005600816410	-0.135858239066	-2.106192455451

**RBiBr<sub>2</sub> (R =2-PhC<sub>6</sub>H<sub>4</sub>)**

Coordinates of structure 1:

C	0.118529937776	1.252792249464	0.069154298097
C	0.262200590017	2.029526682515	-1.099279761708
C	1.176271241533	3.088072233745	-1.150873110244
C	1.947495891918	3.394344016049	-0.030462216218
C	1.790060626921	2.650612977153	1.143571569865
C	0.885985113336	1.591244549217	1.194006641803
C	-0.771914167847	0.068278025819	0.067011738165
C	-0.590211521862	-0.920704668787	-0.920254050252
C	-1.418744215977	-2.044006657297	-0.943503945002
C	-2.419115505619	-2.197493823292	0.020584220810
C	-2.586074170491	-1.230985669030	1.015227599903
C	-1.763322235807	-0.104550150348	1.043265094751
H	-0.409877073230	1.847672597317	-1.943017736019
H	1.268300657881	3.682535881353	-2.060487696581
H	2.663997365268	4.215160957888	-0.066739593267
H	2.391656061077	2.887862604251	2.021415533644
H	0.793971191484	0.988356640626	2.097684862074
H	-1.268556625971	-2.816543177304	-1.700630008765
H	-3.062388413462	-3.078380198178	0.000431403449
H	-3.362855180014	-1.352939799948	1.771338701737
H	-1.900009780003	0.658097866968	1.812556909432
Bi	1.165587524618	-0.613937976077	-2.330458542764
Br	0.786702820453	-2.896060095487	-3.643950528565
Br	2.983587178000	-1.296528156618	-0.531887624346

Coordinates of structure 2:

C	0.144892070747	1.279235293153	0.080507410824
C	0.341245869769	1.987601996761	-1.123113434180
C	1.198794282340	3.090933819799	-1.176442560184
C	1.864549240889	3.510492393473	-0.024681452619
C	1.660787401817	2.829861473167	1.179908332380
C	0.810746007195	1.725602826386	1.233147472037
C	-0.709351186320	0.067479382582	0.097590828347
C	-0.453789316506	-0.970281481303	-0.818344882416
C	-1.259592851835	-2.110838158509	-0.826359713044
C	-2.308285311054	-2.233874161989	0.087434731185
C	-2.550313004390	-1.216544900441	1.015254765633
C	-1.753760172841	-0.072228963186	1.024895188767
H	-0.246044594352	1.708233594735	-2.002744969055
H	1.329645208783	3.631476803028	-2.114286189497
H	2.533454706814	4.370433198810	-0.061256287757
H	2.179162258238	3.155077610166	2.082267536785
H	0.674202578801	1.180672234957	2.167705918556
H	-1.061955432800	-2.912961260741	-1.540165763021
H	-2.934723581799	-3.126890939281	0.079323837685
H	-3.368630904145	-1.312621601769	1.729969148980
H	-1.953097793932	0.731498877806	1.736342625908
Bi	1.391696431099	-0.751726381882	-2.116567225575
Br	0.389246065620	-2.180615035149	-4.113171820231
Br	2.762399337864	-2.577589710574	-0.762509739509

Coordinates of structure 3:

C	0.145142574176	1.271350712340	0.099011229565
C	0.464908326834	1.832481592830	-1.155456444454
C	1.302885448004	2.948745823327	-1.247916729755
C	1.818976813041	3.531946590790	-0.090957365907
C	1.486522440965	3.000073149795	1.159191937269
C	0.658808083696	1.881685847717	1.254648026926
C	-0.672409132300	0.037291506861	0.167432662699
C	-0.322399219446	-1.069105799977	-0.631866651985
C	-1.094553848883	-2.232052824319	-0.592903371750
C	-2.213763172554	-2.303213275017	0.239107293294
C	-2.552779732334	-1.215528375684	1.049473559865
C	-1.783337681894	-0.053307472338	1.021168962575
H	-0.008172420701	1.433763765954	-2.058145241965
H	1.532548809139	3.370167467444	-2.226761638957
H	2.470165010731	4.403448481486	-0.159601459605
H	1.884774635170	3.454652402386	2.066684206632
H	0.423586171400	1.454421912259	2.230162525804
H	-0.809215372070	-3.096096606610	-1.195453523178
H	-2.817330446267	-3.211529917677	0.262177631335
H	-3.424457495385	-1.271865510543	1.702471979967
H	-2.056528000665	0.802823955620	1.640498553336
Bi	1.624884150126	-0.905047947818	-1.778785268081
Br	0.523634417945	-0.743991402561	-4.184782267638
Br	2.099386951271	-3.518687166266	-1.734694845993



Coordinates of structure 4:

C	0.138702972984	1.180936876138	-0.113258288722
C	-0.263996477602	2.133686644078	-1.061939295170
C	0.443098354756	3.326404738148	-1.211939364300
C	1.551735101921	3.591106615101	-0.404189314212
C	1.953445726840	2.653863926061	0.548649592718
C	1.255100795505	1.454578030583	0.688268704890
C	-0.642711477475	-0.064115316251	0.081969152977
C	-0.098294697521	-1.351942276264	-0.072034140159
C	-0.892519342279	-2.475409547379	0.204007371376
C	-2.222920680850	-2.349753314982	0.606299975163
C	-2.773963121603	-1.074001483560	0.724016108230
C	-1.990313399530	0.050129066160	0.466045891571
H	-1.126656703521	1.923361363308	-1.695368305600
H	0.128970571040	4.051458984549	-1.963732760296
H	2.102474589569	4.525146901717	-0.518692418194
H	2.819694123457	2.850730657525	1.180865982398
H	1.565935071605	0.723260499653	1.435822980545
H	-0.487413003075	-3.489361842145	0.079921822473
H	-2.822116184203	-3.236571457431	0.812995666077
H	-3.813818405536	-0.950864347758	1.027891869758
H	-2.415609657339	1.048364285660	0.581977584982
Bi	1.837450659447	-2.172336954539	-0.915793277025
Br	3.534557673369	-0.193869530759	-1.267140654149
Br	0.900444820041	-2.352375607613	-3.379941125331

Coordinates of structure 5:

C	0.032594570915	1.165892199515	-0.247465484574
C	-0.552290804218	2.204874515549	-0.988949836210
C	0.155180191274	3.378587766368	-1.243243288371
C	1.451435887701	3.537832870726	-0.746938215366
C	2.035209598813	2.516456003654	0.004441304404
C	1.332000536278	1.338571635610	0.251297730881
C	-0.715186374827	-0.080010593298	0.030169110229
C	-0.163639710977	-1.360820329175	-0.176008098035
C	-0.902515943599	-2.500759242551	0.172747879131
C	-2.188845048400	-2.400722297008	0.707008146505
C	-2.748697384977	-1.135481236477	0.883635859036
C	-2.019993603682	0.005064137985	0.547733419385
H	-1.557105292826	2.074332106045	-1.392827772202
H	-0.303797953360	4.169989259933	-1.837085751012
H	2.005012001761	4.455635281020	-0.947844636514
H	3.045257064097	2.631971535217	0.397366103123
H	1.787612833405	0.545946316094	0.845630197180
H	-0.486143581374	-3.504484694551	0.013886164836
H	-2.745070834994	-3.298520898881	0.976684928931
H	-3.752793562430	-1.033393460012	1.295866411845
H	-2.451022789452	0.993150717132	0.715713918063
Bi	1.701311806393	-2.061967599465	-1.237096157422
Br	3.495024321147	-1.756549853385	0.696379000396
Br	2.227741383330	-0.083167230049	-2.886397174243

Coordinates of structure 6:

C	0.003345279263	1.220290538661	-0.323161018780
C	-0.606207413928	2.236475781583	-1.076210185384
C	0.054025071761	3.443252803660	-1.303088042971
C	1.324964040555	3.658454411717	-0.764300386768
C	1.935440526898	2.657358835519	-0.007407590980
C	1.283050439205	1.443735582493	0.205631744849
C	-0.706826430987	-0.043449051373	-0.021550909942
C	-0.118809717777	-1.310717846372	-0.203252687916
C	-0.805537060100	-2.457988907232	0.227918907254
C	-2.069735089212	-2.374556095995	0.813251957461
C	-2.669375792826	-1.122701838328	0.956725308358
C	-1.992239914564	0.024177697711	0.546600681905
H	-1.598252517917	2.068025012766	-1.497777037688
H	-0.424080130973	4.218710214141	-1.902790214323
H	1.839288164856	4.604232300500	-0.937538959392
H	2.928880538386	2.816269807197	0.411731396831
H	1.757440104081	0.660566698927	0.798834325460
H	-0.354587294015	-3.451045303715	0.108508298433
H	-2.578538778455	-3.277168631979	1.151882227408
H	-3.659247913495	-1.036021755171	1.405174507408
H	-2.444186538385	1.005713175192	0.697485350539
Bi	1.553529224677	-2.050151932700	-1.542044291006
Br	2.993433053686	-3.114736867164	0.407846913218
Br	3.035505459264	-0.016297720040	-2.317766533975

**RBiI<sub>2</sub> (R =2-PhC<sub>6</sub>H<sub>4</sub>)**

Coordinates of structure 1:

C	0.113105137559	1.259235062587	0.069074932068
C	0.259847717264	2.035185893102	-1.099538854132
C	1.176065863645	3.092108837201	-1.149746541282
C	1.944778135548	3.398334191229	-0.027727589948
C	1.782470878144	2.656960073696	1.147078484843
C	0.876932125590	1.598918158539	1.195988743298
C	-0.777180288886	0.074864462107	0.067199048491
C	-0.596967366003	-0.918165221282	-0.917061645907
C	-1.426597475434	-2.040715704021	-0.932383437558
C	-2.424895906631	-2.190343157687	0.034228724125
C	-2.590726968201	-1.219883389240	1.024987308012
C	-1.767677814472	-0.093808591558	1.045325807491
H	-0.411642929952	1.855190210163	-1.943980924599
H	1.271331882522	3.685454062123	-2.059714289361
H	2.663065424163	4.217612314437	-0.063325207634
H	2.381921653993	2.894322326520	2.026305849768
H	0.782190618895	0.996568665239	2.099669964803
H	-1.281786661057	-2.816054558502	-1.687956989308
H	-3.068111990349	-3.071399780849	0.018191931053
H	-3.366022274788	-1.338198966148	1.783170361874
H	-1.902484695996	0.672996429998	1.810818708758
Bi	1.153642211814	-0.598883662288	-2.341545184917
I	0.741461510125	-3.018027953935	-3.850500440320
I	3.148558522505	-1.329842791430	-0.413854999621

Coordinates of structure 2:

C	0.141711311084	1.286065320487	0.078945704926
C	0.337911143147	1.986202024250	-1.129864982091
C	1.189196164898	3.094096202913	-1.188869102714
C	1.848158608718	3.526780946603	-0.038112950464
C	1.644532100684	2.854248005250	1.171079514222
C	0.800744272576	1.745424470955	1.230208818828
C	-0.707977300151	0.071595311722	0.101934547826
C	-0.448442255573	-0.971946380618	-0.806175099578
C	-1.253014917448	-2.113082563907	-0.808004618073
C	-2.303706932875	-2.231667232795	0.103771288596
C	-2.549823893547	-1.208792536245	1.024543318830
C	-1.754839051451	-0.063727300976	1.027686065425
H	-0.245115342969	1.696627776483	-2.009005996256
H	1.320240504534	3.627753349986	-2.130603346805
H	2.511817744442	4.390576401502	-0.079131150801
H	2.157675251164	3.189812109081	2.072634748557
H	0.664538457301	1.206943316436	2.168550339515
H	-1.053806530269	-2.919660228492	-1.516429063256
H	-2.928976225357	-3.125575628570	0.099327110327
H	-3.369575843074	-1.301269505958	1.738075031001
H	-1.956903612738	0.745239081500	1.732421523460
Bi	1.411537263372	-0.746739601949	-2.090456927888
I	0.336327735259	-2.218100405855	-4.309731496700
I	2.889068658272	-2.718376021803	-0.608089516887

Coordinates of structure 3:

C	0.135337882079	1.282811364237	0.089714163836
C	0.455488914490	1.837660431571	-1.166966881705
C	1.288538949327	2.957176203318	-1.263478215894
C	1.797542216043	3.550531395998	-0.108608506730
C	1.463269635540	3.025274430051	1.143816390928
C	0.641025781510	1.903036637893	1.243401537518
C	-0.675278078989	0.043802468053	0.165655296666
C	-0.300051238644	-1.081079902996	-0.595707931673
C	-1.064588194183	-2.248128811048	-0.539867213516
C	-2.196975522312	-2.307914640343	0.274799847456
C	-2.561505330715	-1.201792917027	1.047881804835
C	-1.801434297187	-0.034170548183	1.000585890839
H	-0.009504175891	1.428859016365	-2.069253818101
H	1.520309996371	3.372415524170	-2.244543631584
H	2.444950458652	4.424625953334	-0.180488175683
H	1.855770156230	3.487946244596	2.049741734222
H	0.404250974807	1.480697925186	2.220702026160
H	-0.764455754434	-3.125607875359	-1.115424035093
H	-2.792081328987	-3.221384229399	0.311210765923
H	-3.444416774988	-1.247913630997	1.686378094084
H	-2.091700698034	0.836284171489	1.591395797796
Bi	1.649934841195	-0.905026811385	-1.747476354640
I	0.444785139083	-0.748172818666	-4.350912877505
I	2.282063759038	-3.707502670859	-1.607851948137

Coordinates of structure 4:

C	0.134626870410	1.187733171369	-0.121465893324
C	-0.213041635607	2.084947165299	-1.141825915992
C	0.478781380853	3.286882581860	-1.292871123024
C	1.512612387523	3.617388836245	-0.413451133435
C	1.857970652501	2.735265451408	0.611661098632
C	1.179038547728	1.525033392007	0.750574156980
C	-0.631322386183	-0.066889346443	0.082759401716
C	-0.063096464150	-1.347734830040	-0.032040359602
C	-0.837639006334	-2.476345441725	0.279539751488
C	-2.167709755980	-2.358834705242	0.683040917790
C	-2.744501556433	-1.090628394501	0.756959378400
C	-1.981189485123	0.037827341022	0.461951738772
H	-1.020213025561	1.825276171612	-1.828125672367
H	0.209587174784	3.969074087603	-2.100193492786
H	2.048415628101	4.559992743985	-0.527749009358
H	2.665278445771	2.984468087482	1.301183832024
H	1.442657109290	0.836123939288	1.554810795883
H	-0.418106419474	-3.485013259641	0.176791352198
H	-2.750183081697	-3.249399435195	0.919744409450
H	-3.787233053376	-0.977397991819	1.054711757371
H	-2.422908677645	1.032313075243	0.544379581799
Bi	1.913354855239	-2.103734273413	-0.862343191658
I	3.507776887812	0.125519096995	-1.640033272830
I	0.768321917550	-2.849440553399	-3.383305348126

Coordinates of structure 5:

C	0.018932956756	1.156209046646	-0.246352412118
C	-0.575084780026	2.125200742546	-1.070444534698
C	0.107739470464	3.297593027437	-1.389855243636
C	1.388149014827	3.525464736899	-0.879371835823
C	1.978341599233	2.576179223780	-0.043520187111
C	1.298213607945	1.400731141859	0.270702298478
C	-0.701149303522	-0.093687812640	0.085058970534
C	-0.137560954746	-1.373918999758	-0.090617662001
C	-0.871643091429	-2.512398478948	0.273284522635
C	-2.165064181577	-2.412272226745	0.790360994749
C	-2.734476215341	-1.148448624600	0.942398755783
C	-2.010328466869	-0.009500946407	0.591521969565
H	-1.565285254598	1.937633606112	-1.487550119294
H	-0.357367550757	4.033170915594	-2.047388379149
H	1.923014508833	4.441033642071	-1.133602860669
H	2.975154188724	2.745651308356	0.363921002805
H	1.758117744736	0.667304519513	0.932461699208
H	-0.443783510821	-3.514931478580	0.141422225839
H	-2.717973392754	-3.309750730989	1.067967681245
H	-3.742502863626	-1.045715925148	1.344755158642
H	-2.451811111759	0.978431264976	0.731414339649
Bi	1.779017882000	-2.086967487059	-1.062359747466
I	3.816328341550	-1.435228552990	0.863304130149
I	2.112298672758	-0.139355001924	-3.112807007315



Coordinates of structure 6:

C	-0.001934062045	1.225528205445	-0.323577858753
C	-0.475568620928	1.962721063409	-1.417408318294
C	0.114703592870	3.180453460161	-1.760082624891
C	1.173646464202	3.682561665452	-1.001686566956
C	1.646062537851	2.957591750900	0.093568938238
C	1.068348276727	1.732482235841	0.424878992596
C	-0.659349258683	-0.046907538150	0.084156425206
C	-0.151328707461	-1.316963128663	-0.242550993097
C	-0.809648666643	-2.465616405235	0.227874942237
C	-1.974494312607	-2.369249751227	0.989547136531
C	-2.491828379593	-1.110359450457	1.295624096589
C	-1.835494086863	0.035456979180	0.848592074728
H	-1.315361959254	1.576886494413	-1.998021609028
H	-0.257822442478	3.740256456175	-2.618644011837
H	1.631199139391	4.635995548934	-1.265850193770
H	2.480570454066	3.338335858052	0.683053654681
H	1.443079525203	1.158422636167	1.272801360445
H	-0.405709038327	-3.458520612326	0.010874931101
H	-2.468906111894	-3.273166093542	1.346270722265
H	-3.401273734573	-1.017770589354	1.890158566024
H	-2.226018675962	1.022571680236	1.100651138564
Bi	1.437704528517	-1.854910852554	-1.784437765312
I	2.778730320190	-3.764016472404	-0.119267739845
I	3.381970528296	0.230643769545	-1.901821537423

Selected geometries from potential energy surface of halogen substituted R<sub>2</sub>BiX compounds along the C-C-C-C dihedral scan.

**RBiCl<sub>2</sub> (R =2-PhC<sub>6</sub>H<sub>4</sub>)**

Coordinates of structure 1:

C	0.120020090	1.247940601	0.066203983
C	0.262380137	2.029158668	-1.098691705
C	1.180857834	3.083771341	-1.148595617
C	1.958176773	3.381142116	-0.029812365
C	1.802690526	2.631981855	1.140890100
C	0.893494471	1.576885567	1.189671744
C	-0.773952488	0.065657604	0.063051402
C	-0.589279619	-0.924281620	-0.921997382
C	-1.415802292	-2.049240581	-0.945989259
C	-2.419267897	-2.201855692	0.015251930
C	-2.590024056	-1.233317815	1.007365537
C	-1.767753475	-0.106260013	1.036985370
H	-0.410627226	1.851623385	-1.942572610
H	1.271950565	3.682669568	-2.055442247
H	2.678220371	4.198934867	-0.064967428
H	2.409257472	2.861683667	2.017381301
H	0.802287012	0.969726367	2.090584202
H	-1.259589734	-2.823270039	-1.700178690
H	-3.061560405	-3.083480656	-0.004611877
H	-3.369290922	-1.354524703	1.761064951
H	-1.906413143	0.656365877	1.805942815
Bi	1.155635922	-0.629936842	-2.343316680
Cl	0.830311963	-2.841416797	-3.455833973
Cl	2.879555430	-1.187529816	-0.647679742

Coordinates of structure 2:

C	0.108927764875	1.265894900835	0.062615446466
C	-0.011471182550	2.232515076596	-0.953334396597
C	0.885612805120	3.301356109407	-1.030357972449
C	1.915786513834	3.417178109837	-0.094839480638
C	2.048249149273	2.460432240952	0.914102654812
C	1.152651296086	1.391965701297	0.994027824229
C	-0.792777551159	0.076093950027	0.076939627653
C	-0.467314636604	-1.002276064022	-0.763753944384
C	-1.279744731371	-2.136729428249	-0.804637705456
C	-2.418633923255	-2.201460725841	0.002393622655
C	-2.743058257589	-1.133736486453	0.843966928794
C	-1.934033454660	0.004528057933	0.884590768337
H	-0.823738626844	2.142122636466	-1.677356199275
H	0.776104875120	4.045040340524	-1.820705002318
H	2.618674517926	4.248720372368	-0.155387740125
H	2.858133579212	2.539852642448	1.640011718065
H	1.271353012862	0.631288042930	1.766034687896
H	-1.020672455534	-2.968847511363	-1.462001395969
H	-3.054834813526	-3.087357454590	-0.024917007311
H	-3.634042404359	-1.185529659768	1.470808104721
H	-2.189012272059	0.841098103519	1.537346708599
Bi	1.428373962065	-0.698114257197	-1.952289942838
Cl	1.053800652757	-2.697788789891	-3.382193377464
Cl	2.932943490379	-1.683818997765	-0.236360167403

Coordinates of structure 3:

C	0.110932240797	1.294878453839	-0.011498914245
C	-0.329558373323	2.532199098745	-0.510199025153
C	0.532235450957	3.627628742563	-0.554482610481
C	1.851134614371	3.511235769275	-0.103128185045
C	2.299907330540	2.293757727218	0.408756402690
C	1.435155533674	1.195343031577	0.463428004359
C	-0.767370126168	0.101189761337	-0.016931534316
C	-0.295823374333	-1.108615140981	-0.564568713375
C	-1.111475624979	-2.242268477594	-0.563043389384
C	-2.397814807428	-2.181085540106	-0.022764922552
C	-2.878202841644	-0.977923620267	0.502054764242
C	-2.072221876493	0.159675053934	0.498355114184
H	-1.348968657164	2.619974621110	-0.887633396324
H	0.176734423605	4.577748762563	-0.954588236833
H	2.521251719060	4.370129969651	-0.145001983496
H	3.317153448968	2.196997356238	0.788414338519
H	1.764960898636	0.270979806416	0.947103081931
H	-0.749346310166	-3.171832770513	-1.005316466085
H	-3.028654243806	-3.070977732412	-0.018950937627
H	-3.883683003812	-0.927416397411	0.920676358235
H	-2.439838158264	1.095352109348	0.922697345647
Bi	1.734743425696	-1.071192425790	-1.567102790501
Cl	1.263111922059	-3.084909718531	-2.955031527136
Cl	2.976913699217	-2.208441530207	0.263460982747

Coordinates of structure 4:

C	0.163267568262	1.283463347131	0.144287725755
C	-0.380340074441	2.583306884715	0.208442927537
C	0.410766989442	3.720505512208	0.061753660852
C	1.782809583853	3.613011296554	-0.177082002353
C	2.357954798847	2.344140160585	-0.207346336942
C	1.559679054731	1.210926561953	-0.047035747672
C	-0.707970124651	0.078656314851	0.060365231430
C	-0.212358214432	-1.204265638558	-0.308018921629
C	-1.084538302074	-2.297705608001	-0.369963632679
C	-2.457795683602	-2.146257021725	-0.176016344212
C	-2.971974229040	-0.864233714520	0.009654019325
C	-2.110084892494	0.224722106592	0.101341575869
H	-1.449225376723	2.724380547589	0.356445735311
H	-0.056429392558	4.704394909680	0.119498608275
H	2.395671556911	4.504916528840	-0.305266413286
H	3.436300242612	2.226509650925	-0.319576080870
H	2.085910831188	0.276726539509	0.178570657127
H	-0.692814370687	-3.281531075278	-0.634585917392
H	-3.118381156462	-3.012281856181	-0.226513072663
H	-4.048590984411	-0.703881671017	0.080676002751
H	-2.550615780085	1.205025003204	0.274359400992
Bi	1.769970202162	-1.498722428800	-1.390977988651
Cl	1.330452602024	-3.833536989505	-2.143681023315
Cl	3.229612461627	-2.055842450750	0.545371696442

**RBiBr<sub>2</sub> ( R = 2-PhC<sub>6</sub>H<sub>4</sub>)**

Coordinates of structure 1:

C	0.118529937776	1.252792249464	0.069154298097
C	0.262200590017	2.029526682515	-1.099279761708
C	1.176271241533	3.088072233745	-1.150873110244
C	1.947495891918	3.394344016049	-0.030462216218
C	1.790060626921	2.650612977153	1.143571569865
C	0.885985113336	1.591244549217	1.194006641803
C	-0.771914167847	0.068278025819	0.067011738165
C	-0.590211521862	-0.920704668787	-0.920254050252
C	-1.418744215977	-2.044006657297	-0.943503945002
C	-2.419115505619	-2.197493823292	0.020584220810
C	-2.586074170491	-1.230985669030	1.015227599903
C	-1.763322235807	-0.104550150348	1.043265094751
H	-0.409877073230	1.847672597317	-1.943017736019
H	1.268300657881	3.682535881353	-2.060487696581
H	2.663997365268	4.215160957888	-0.066739593267
H	2.391656061077	2.887862604251	2.021415533644
H	0.793971191484	0.988356640626	2.097684862074
H	-1.268556625971	-2.816543177304	-1.700630008765
H	-3.062388413462	-3.078380198178	0.000431403449
H	-3.362855180014	-1.352939799948	1.771338701737
H	-1.900009780003	0.658097866968	1.812556909432
Bi	1.165587524618	-0.613937976077	-2.330458542764
Br	0.786702820453	-2.896060095487	-3.643950528565
Br	2.983587178000	-1.296528156618	-0.531887624346

Coordinates of structure 2:

C	0.103542714214	1.274658985981	0.065200509104
C	-0.015851922347	2.234071197473	-0.958147803211
C	0.878969549064	3.304353977043	-1.039664827242
C	1.906235721120	3.428779620741	-0.101913846604
C	2.037466936775	2.479881834845	0.914521807413
C	1.143543465530	1.410184684439	0.999813043259
C	-0.793974267683	0.081814137029	0.082693571722
C	-0.465938244964	-0.996149580059	-0.757829748654
C	-1.275585338869	-2.132382976325	-0.797209985044
C	-2.412120746294	-2.200602912253	0.012582768178
C	-2.737856552177	-1.134353839330	0.855586767912
C	-1.932825557376	0.006645972510	0.893354873429
H	-0.825469539274	2.136296768089	-1.684108419092
H	0.770211213120	4.042193358639	-1.835538997623
H	2.607723915226	4.261170491390	-0.166574228694
H	2.844839961288	2.566495646496	1.642393912383
H	1.260248182901	0.656557158504	1.779046144466
H	-1.017162223521	-2.964093719265	-1.455508763740
H	-3.045385516691	-3.088608828908	-0.013570699622
H	-3.626647487512	-1.189437961010	1.485213245185
H	-2.188919773336	0.842976271369	1.545977970360
Bi	1.442110426705	-0.676056705783	-1.925887425933
Br	1.021346920455	-2.702598920168	-3.580871698415
Br	3.002775473647	-1.839367751448	-0.124854409537

Coordinates of structure 3:

C	0.104354221902	1.301638109509	-0.005096318212
C	-0.332696344078	2.533367466800	-0.519959601998
C	0.529658808771	3.628300535302	-0.569504500130
C	1.845190319347	3.516919050143	-0.106999135443
C	2.290316589575	2.305335212646	0.421618377954
C	1.425067457327	1.207495621234	0.481087405693
C	-0.771096536060	0.105527893849	-0.007600653574
C	-0.295516362881	-1.104600547914	-0.551511872084
C	-1.107184458643	-2.240884657455	-0.544482522947
C	-2.393513994100	-2.181823898208	-0.004263088654
C	-2.878875086510	-0.977860098377	0.514245980041
C	-2.076631861742	0.162238321603	0.505896898815
H	-1.349047949763	2.616764737465	-0.906474474535
H	0.177437966897	4.573915301655	-0.982907088065
H	2.515708736979	4.375251653361	-0.153687259509
H	3.304858445364	2.212330705021	0.809301992805
H	1.750987128208	0.288052927788	0.977007542834
H	-0.743526056761	-3.171825111172	-0.982838028954
H	-3.020937670128	-3.074071285439	0.003425732774
H	-3.885038542783	-0.928758936327	0.931319831996
H	-2.447405244472	1.098990766249	0.925127957685
Bi	1.731483594641	-1.033757222672	-1.563176859628
Br	1.234501352294	-3.091697145899	-3.165709581282
Br	3.073182796618	-2.318422489163	0.329883024418



Coordinates of structure 4:

C	0.155633071390	1.290909706820	0.146676196202
C	-0.387460909698	2.591196389222	0.205556158391
C	0.406373867168	3.726968867026	0.062839388320
C	1.780059084132	3.617439765231	-0.166650917787
C	2.354143637665	2.348103227374	-0.193153730480
C	1.552899071512	1.216475821677	-0.036502525177
C	-0.713522516452	0.085404934668	0.062410195438
C	-0.215622175654	-1.197476046322	-0.304949464049
C	-1.084771941422	-2.293348348719	-0.357100513608
C	-2.457875047966	-2.144318580579	-0.161586125770
C	-2.975442018863	-0.862512404792	0.016952680385
C	-2.115991014458	0.228581381927	0.103957880502
H	-1.457211776112	2.733277882185	0.346300252677
H	-0.059689846269	4.711633599490	0.116204288628
H	2.394760975340	4.508623141693	-0.290955111069
H	3.432953232268	2.228602361302	-0.298791664171
H	2.074343927431	0.279865525562	0.193376038425
H	-0.692488784682	-3.278506243983	-0.616012562247
H	-3.115994738861	-3.012487382093	-0.206696831500
H	-4.052472629463	-0.704627236795	0.086949070415
H	-2.557786392012	1.208783489041	0.274255203855
Bi	1.759913550101	-1.458586577238	-1.414847554472
Br	1.304916778840	-3.908054262546	-2.338632682077
Br	3.351609906064	-2.113522100151	0.605106089167

## **RBiI<sub>2</sub> (R =2-PhC<sub>6</sub>H<sub>4</sub>)**

Coordinates of structure 1:

C	0.113174200573	1.259270883965	0.069021359132
C	0.259806942479	2.035352393350	-1.099520765704
C	1.175991589100	3.092299091408	-1.149700377322
C	1.944769547085	3.398473590069	-0.027696491140
C	1.782563175582	2.656976864023	1.147053686356
C	0.877038883853	1.598911337536	1.195928961365
C	-0.777152786094	0.074926940328	0.067121015451
C	-0.596894801449	-0.918125670688	-0.917081469269
C	-1.426459647178	-2.040731854770	-0.932404570347
C	-2.424829779744	-2.190383547146	0.034132359215
C	-2.590722581840	-1.219879400336	1.024857455302
C	-1.767657661553	-0.093803026750	1.045230900194
H	-0.411751539758	1.855410685870	-1.943941688833
H	1.271162385509	3.685739363741	-2.059633708333
H	2.662998391614	4.217821485876	-0.063254478702
H	2.382058579109	2.894286356939	2.026280581202
H	0.782388364045	0.996457801979	2.099568413713
H	-1.281296894192	-2.816125910672	-1.687878620275
H	-3.068004002513	-3.071485183425	0.018104674748
H	-3.366049097122	-1.338177858233	1.783030675199
H	-1.902488967526	0.672991084766	1.810752759724
Bi	1.153430621565	-0.599128146929	-2.341339728121
I	0.740988557692	-3.018308389692	-3.850375325255
I	3.148213830763	-1.330341981210	-0.413551858300

Coordinates of structure 2:

C	0.097502100638	1.286133147136	0.046593985197
C	-0.070449786138	2.289996101162	-0.925082755080
C	0.821137434505	3.362367069334	-1.000911880997
C	1.892240944025	3.446348098230	-0.107813037871
C	2.069558319833	2.455702439309	0.859867195864
C	1.177082373607	1.383724647444	0.941490102518
C	-0.801925298685	0.094096843856	0.068007330406
C	-0.450057793100	-1.008705360521	-0.729850886685
C	-1.254798298502	-2.148730798036	-0.751457938859
C	-2.409314947749	-2.196438924904	0.033537173258
C	-2.758587336739	-1.105954961450	0.835044484619
C	-1.959122924248	0.039172246915	0.854126628950
H	-0.909575861341	2.220309617254	-1.619537843957
H	0.677506460422	4.134035405146	-1.758242304711
H	2.591209634809	4.281122645507	-0.170131882025
H	2.908610475570	2.511852133884	1.554040839197
H	1.326628330212	0.598068078430	1.682633847767
H	-0.981264427967	-2.998103903016	-1.380675227974
H	-3.038352799428	-3.087770650932	0.020793268248
H	-3.660372212493	-1.145726901199	1.447042862629
H	-2.231245439065	0.893787002741	1.475847938079
Bi	1.485091642698	-0.693754872008	-1.860938489833
I	1.024530439745	-2.790191142321	-3.764000517219
I	3.135246279392	-2.018911051961	0.084320868479

Coordinates of structure 3:

C	0.100639256010	1.311973716838	-0.004821294457
C	-0.338863173722	2.540937137858	-0.523700565847
C	0.520908457128	3.637968186448	-0.574608541954
C	1.836112894912	3.531205602763	-0.109896106819
C	2.283344156922	2.322285592836	0.423051210536
C	1.420324078589	1.223002316747	0.484600577891
C	-0.770274294321	0.112521769834	-0.004838698444
C	-0.293132758793	-1.098701070812	-0.545128395927
C	-1.101213182707	-2.237195739058	-0.527017417191
C	-2.386508147365	-2.179186198265	0.015463275561
C	-2.875142323714	-0.973682197237	0.527109003815
C	-2.075656251374	0.167943654593	0.509933647473
H	-1.354558208408	2.620711568980	-0.912676376857
H	0.166891704316	4.581616136138	-0.990975938951
H	2.504520859830	4.391101124641	-0.158356773531
H	3.297518648062	2.232477873296	0.812522364399
H	1.746087936792	0.306060227341	0.985920085510
H	-0.737894756023	-3.170092396062	-0.961649196469
H	-3.010273918174	-3.073926959714	0.030108877788
H	-3.880851703949	-0.924593883673	0.945226363835
H	-2.447663965993	1.106402077397	0.924272016118
Bi	1.741310126486	-1.022391005629	-1.554660631642
I	1.175314599638	-3.126384085479	-3.431332564243
I	3.160337275860	-2.477626539782	0.476158839406

Coordinates of structure 4:

C	0.150607301078	1.300622146119	0.152107283905
C	-0.390989947718	2.601788091964	0.200263006173
C	0.406074762724	3.735591502282	0.058872861812
C	1.781809157401	3.622625657297	-0.157504789101
C	2.353819708726	2.352248609135	-0.172657949393
C	1.549346028003	1.222288848242	-0.018224365809
C	-0.717712044626	0.095251210200	0.066002902012
C	-0.217219251493	-1.188255570885	-0.295852413055
C	-1.082713223981	-2.287296415371	-0.332309243166
C	-2.456236433194	-2.139062691207	-0.140914830648
C	-2.977827995461	-0.856139360623	0.018341023833
C	-2.120811313901	0.237449320718	0.097594535963
H	-1.461750526301	2.746290046766	0.331180268604
H	-0.058783415435	4.721305727940	0.102774776751
H	2.399011528513	4.512223778589	-0.280975319331
H	3.433452646738	2.229961748919	-0.267186295162
H	2.068945584242	0.286721669824	0.223505240390
H	-0.687632971316	-3.275093552616	-0.577328820449
H	-3.111653436765	-3.009816873039	-0.174964382699
H	-4.055553392834	-0.699812178727	0.080710958262
H	-2.564489124831	1.218792741322	0.256273891254
Bi	1.756592339328	-1.424418276322	-1.424064509316
I	1.223160734205	-3.971668479952	-2.655468683301
I	3.461830596896	-2.229170790573	0.744528612471

Optimized structure of four lowest energy conformations from GFN2-XTB simulations

**R<sub>2</sub>BiCH<sub>3</sub>**

Structure 1.

C	-0.324635579186	-3.681371532716	-0.676716312804
C	0.850139127037	-2.987823065177	-0.390190763244
C	1.191762712423	-1.829771993253	-1.104675350850
C	0.333944904410	-1.397617887321	-2.130241617184
C	-0.841801710322	-2.092483902605	-2.419397924427
C	-1.174481541393	-3.235767958462	-1.691663501418
H	-2.094150500241	-3.779134164896	-1.914797760100
H	-1.496948023669	-1.741339541241	-3.218259375713
H	0.610314274623	-0.524453307154	-2.725546180577
C	2.416356243764	-1.063554466520	-0.764449885694
C	3.663249164880	-1.708601971853	-0.761536795364
C	4.826301796717	-1.012240920915	-0.431267274459
C	4.751833813577	0.338368836407	-0.088610528067
C	3.509515447364	0.980647516896	-0.068260613765
C	2.334644526916	0.296375910007	-0.397939855650
Bi	0.288845349927	1.317693800991	-0.258401871753
C	-0.356278214208	-0.173667829796	1.342648426407
C	0.599008602998	-0.715013845438	2.209255442468
C	0.271744496283	-1.748512097220	3.089262466021
C	-1.027441179977	-2.261660694049	3.101683845002
C	-1.993668240840	-1.718825155044	2.257842178170
C	-1.677218175305	-0.660825365171	1.386949956971
C	-2.739631548308	-0.073658092157	0.537981179530
C	-3.577584472877	-0.881862225562	-0.246581661181

C	-4.564574408405	-0.316204390458	-1.053712016664
C	-4.740180378921	1.069968261994	-1.085177529554
C	-3.925114950286	1.886041736507	-0.298524530049
C	-2.935277005460	1.318556807507	0.505597121017
H	-2.331012138414	1.953576697641	1.158983518824
H	-4.067363408190	2.968450130453	-0.301439159076
H	-5.513725114240	1.511795710260	-1.715401608660
H	-5.198094480034	-0.960104514105	-1.666666761412
H	-3.423678426009	-1.962442191844	-0.241883321232
H	-3.018175085948	-2.096323027121	2.284810500634
H	-1.290724743170	-3.077505608622	3.777602476996
H	1.033074121896	-2.160235472731	3.754859848978
H	1.629019058807	-0.352764715598	2.174330154995
C	1.049428422251	2.844870178265	1.276423663921
H	0.185306303032	3.316671680034	1.761233406531
H	1.658701695588	2.323360287395	2.023437982593
H	1.645770529852	3.613461037248	0.768547088025
H	3.465120195392	2.029754065578	0.232260751423
H	5.656982277916	0.889914455343	0.172923647387
H	5.789987733026	-1.524720840627	-0.444521303403
H	3.715847271684	-2.763849555625	-1.038258057754
H	1.496566728582	-3.318555050733	0.424374788171
H	-0.583556473540	-4.567620728511	-0.095499884010

Structure 2.

C	1.835600719847	1.568428091894	-2.354238883747
C	2.161814201390	0.456948471924	-1.575633178366
C	2.225929394112	0.556220793674	-0.176858765683
C	1.950067365865	1.798382973966	0.421352427243
C	1.633774950173	2.913086991198	-0.357985652042

C	1.575879925063	2.800878790575	-1.748768342807
H	1.320590564359	3.668540052235	-2.358983862145
H	1.433460603576	3.871723572560	0.123857910832
H	2.018067993735	1.890238539907	1.507490267604
C	2.590931258122	-0.615920247425	0.661105200352
C	3.850047849898	-1.213766281975	0.497229650860
C	4.229126344595	-2.301039780550	1.285002888945
C	3.347372238740	-2.802208171073	2.243114001445
C	2.082723337332	-2.223913152073	2.393328356566
C	1.683711558407	-1.140982230420	1.603236733727
Bi	-0.438212137285	-0.300599908319	1.660090820837
C	-0.912351642422	-1.370849302761	-0.302451907003
C	-0.285008946509	-2.587969385972	-0.588425713830
C	-0.618367146508	-3.325565001021	-1.726255361560
C	-1.602680657367	-2.849353634043	-2.594713157420
C	-2.233945007487	-1.636933689548	-2.325274024785
C	-1.888159972101	-0.880061900046	-1.192068473607
C	-2.550428049269	0.427815003938	-0.967469671088
C	-1.777120377105	1.586354519005	-0.782797488952
C	-2.384066278695	2.823833259189	-0.567227363380
C	-3.776466580944	2.925057093326	-0.531149126432
C	-4.556715822902	1.781857503705	-0.723874698450
C	-3.949169526454	0.544639208843	-0.943925091647
H	-4.560037673167	-0.349972813613	-1.080989706066
H	-5.645898183080	1.853327667679	-0.697505216698
H	-4.253528711326	3.891183814953	-0.358589821041
H	-1.763363411324	3.712185057763	-0.435519946377
H	-0.690060783076	1.517376141112	-0.849734285759
H	-2.989115660994	-1.248330492567	-3.012514699927
H	-1.873256572943	-3.417812250737	-3.486312693259



H	-0.113786960469	-4.271705449052	-1.930253604393
H	0.477045994961	-2.977146473701	0.092007630538
C	-1.223939204889	-2.076764923266	2.883420637715
H	-0.865492077759	-2.006126381333	3.918090492562
H	-2.320882237427	-2.037999878006	2.871787474570
H	-0.880761281184	-3.009664636579	2.420642373650
H	1.393452941928	-2.651142856289	3.125353735674
H	3.636712868026	-3.650019074783	2.867380449977
H	5.214086568528	-2.751839997572	1.153436099472
H	4.539871414360	-0.806492777712	-0.245518999595
H	2.349369646597	-0.508887010731	-2.047780614106
H	1.775546163068	1.469890153719	-3.439617802401

Structure 3.

C	0.313735768869	2.852982388592	1.653228181317
C	-0.578434809735	1.805257924510	1.419359228777
C	-1.799148392904	2.031516368434	0.759663518667
C	-2.111862089292	3.342546629370	0.365077832944
C	-1.222026455959	4.390320621197	0.602863142922
C	-0.003186497101	4.148696772559	1.242787584914
H	0.694276505070	4.968461763059	1.422102774079
H	-1.476405819514	5.400359997906	0.277132617261
H	-3.053321938846	3.530590844191	-0.154466492587
C	-2.726489012424	0.907502733126	0.475306685732
C	-4.072489422073	1.008389345802	0.865531734870
C	-4.969295569118	-0.030393037604	0.618238930084
C	-4.530559433560	-1.182447877075	-0.036079175111
C	-3.196195760803	-1.282846118649	-0.441679156782
C	-2.280041356746	-0.253289039285	-0.195353081032
Bi	-0.145239573072	-0.320682179578	-1.017810248659

C	0.689093889922	-1.367011695719	0.836976316138
C	-0.157867782256	-2.113354524910	1.663568842953
C	0.303999381144	-2.664924657908	2.861162619375
C	1.628936672534	-2.461003670797	3.253185482391
C	2.484186836125	-1.718960033733	2.440448381351
C	2.031332358572	-1.178384191782	1.223918790123
C	2.966672323608	-0.405637926484	0.372245230581
C	3.699544586360	0.672966647900	0.891780604258
C	4.552577035512	1.415985637989	0.075348449627
C	4.697484900132	1.087561374632	-1.275007726870
C	3.988001589852	0.006693635352	-1.801952938542
C	3.130082499288	-0.731794931746	-0.985484561982
H	2.605557705720	-1.601971487593	-1.387975533248
H	4.107424809714	-0.267710859768	-2.851332641228
H	5.364751388370	1.669711666842	-1.912497612318
H	5.102542514376	2.260751773682	0.493695462748
H	3.576364174164	0.939707117548	1.943506916261
H	3.525862688550	-1.570321882964	2.732585227839
H	1.997276394782	-2.882320807472	4.189812995585
H	-0.373144171270	-3.245246093134	3.491325203185
H	-1.205703283771	-2.248824224354	1.384260850850
C	-0.474302366747	-2.320209734366	-2.097158362102
H	-0.779112366351	-3.082377969476	-1.370796557790
H	-1.240008246997	-2.197833458219	-2.873559836673
H	0.473133962002	-2.620507888197	-2.563387856786
H	-2.874322700265	-2.183238117110	-0.969448148931
H	-5.225416344816	-2.000676725346	-0.236352937895
H	-6.008163660841	0.058663917999	0.940443544163
H	-4.406954399890	1.905070867594	1.392139501922
H	-0.343702678341	0.802249972119	1.780956204563

H	1.257665148028	2.652302132867	2.162361013055
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Structure 4.

C	-1.668477227097	-1.706109641983	-1.927777664675
C	-1.770405517810	-0.514794488306	-1.206019743082
C	-2.752006484046	-0.357334288379	-0.212367094041
C	-3.637355641945	-1.420989681503	0.026447766187
C	-3.531725427020	-2.613282486750	-0.690423994292
C	-2.543902397569	-2.762265558461	-1.667633749233
H	-2.462513462936	-3.694836034329	-2.228210098420
H	-4.220230596617	-3.433907466099	-0.480076658904
H	-4.400601589981	-1.313175772519	0.800068524240
C	-2.843327705928	0.903436933059	0.565726964941
C	-4.070597999931	1.584498064838	0.633289210912
C	-4.186745441831	2.780551412612	1.340582733951
C	-3.073975832051	3.306771077390	1.997923328237
C	-1.855260884915	2.622389843501	1.953398856273
C	-1.719166331823	1.422558589455	1.244819790584
Bi	0.192009694162	0.172191322824	1.368999438237
C	1.202557749327	1.196788646118	-0.410557271175
C	0.732581457283	2.431594521104	-0.872366176466
C	1.393203634255	3.117642750999	-1.895293184265
C	2.543392379574	2.570040325066	-2.466742891644
C	3.018828139482	1.338480119155	-2.018814446009
C	2.351308202922	0.633092787071	-1.001789011806
C	2.876640859078	-0.686131577794	-0.567479574682
C	2.051468288240	-1.824490607967	-0.573253014999
C	2.542770919931	-3.065883665436	-0.166791646510
C	3.868024667448	-3.192017424312	0.254938633891
C	4.700870524524	-2.070324731991	0.258442739532

C	4.210640063088	-0.830340501509	-0.153637865249
H	4.858787386372	0.048135828641	-0.138188687008
H	5.736905490952	-2.159894123768	0.589187978695
H	4.251595082805	-4.161278303617	0.576884283888
H	1.887329520393	-3.938412243771	-0.185095591173
H	1.023062955950	-1.738776947509	-0.929927614177
H	3.907002295918	0.896477189473	-2.475377295036
H	3.066575634561	3.097507538861	-3.266154471369
H	1.010875830377	4.079344097784	-2.241906253988
H	-0.157700733696	2.875102021986	-0.419841837152
C	1.228133181351	1.623513363170	2.813238453817
H	2.251757437928	1.261261383202	2.972240360392
H	1.258087997766	2.622969513167	2.364789479692
H	0.690162590124	1.643588625760	3.769352276152
H	-1.000269938624	3.035436622833	2.492856184230
H	-3.153114900208	4.245147389706	2.549946636437
H	-5.144186732299	3.303635832005	1.371962178174
H	-4.933576282488	1.178193913662	0.101170976601
H	-1.101933321328	0.318162089783	-1.433744382608
H	-0.906615533667	-1.802513257224	-2.704244577100

## **R<sub>2</sub>BiCl**

Structure 1.

C	-2.342817423852	-0.968899038111	2.861077416925
C	-1.074396394544	-1.508336342962	2.654499827167
C	-0.715650437771	-2.036296215460	1.404988423652
C	-1.681085579602	-2.042005312909	0.378752647238
C	-2.951989170252	-1.495228125576	0.584903782421
C	-3.282344120221	-0.952241277964	1.826026784907
H	-4.270788895667	-0.520993874380	1.988739322468

H	-3.685024770800	-1.504735403977	-0.223332636751
H	-1.450813733052	-2.540410059875	-0.567604083340
C	0.669031923423	-2.490473858494	1.132965701212
C	1.304741813585	-3.437866885932	1.948920405681
C	2.618128984540	-3.826270103589	1.681596601533
C	3.311140024970	-3.258336863189	0.609983454645
C	2.691283923514	-2.293768855028	-0.191399806394
C	1.375600531034	-1.901881338666	0.064387480006
Bi	0.302065282866	-0.265800405875	-1.122895017719
Cl	2.437882393834	0.671265025682	-2.068676091218
C	0.239228434950	1.075200157259	0.717520859051
C	1.180531705055	0.922997177252	1.739216408833
C	1.056548787981	1.628714051557	2.937296500237
C	-0.029718786841	2.487013109848	3.126318733887
C	-0.963885568633	2.660870292011	2.107135917955
C	-0.829238281450	1.977626829062	0.885419172013
C	-1.798152981689	2.223583457831	-0.208279711472
C	-3.183361299319	2.174607439063	0.015658231805
C	-4.083209287732	2.382182502520	-1.029441400316
C	-3.615934531631	2.650225245844	-2.319439078403
C	-2.241539843210	2.722124014969	-2.553372433487
C	-1.340802369521	2.514357818209	-1.507106532586
H	-0.266353035359	2.621464945614	-1.682913862890
H	-1.865464103731	2.954215132189	-3.550897978035
H	-4.321051493724	2.811319862881	-3.136252957869
H	-5.156855561949	2.328697082327	-0.837943412488
H	-3.550317184625	1.942674541073	1.016471168336
H	-1.795085188754	3.357408612454	2.238347663500
H	-0.140085475560	3.035534390997	4.063476705412
H	1.802458526114	1.502904139920	3.725007572843

H	2.012627967931	0.227144601370	1.610667280819
H	3.248975128112	-1.818734214908	-1.002157331064
H	4.339491237157	-3.559589424974	0.402487300354
H	3.101773904016	-4.574655333428	2.311908132882
H	0.757635886412	-3.880993303796	2.784076147562
H	-0.329048334728	-1.478138409153	3.450569898555
H	-2.593868601281	-0.538397781685	3.831637792136

Structure 2.

C	4.910312347249	0.985169291639	0.167009736088
C	4.049821497431	0.277304090551	-0.672433092188
C	3.091514649606	-0.600765037895	-0.140982530173
C	3.031196179405	-0.764981449961	1.255076606851
C	3.894925640050	-0.058123380615	2.093897066658
C	4.833471153113	0.822926358595	1.553183575432
H	5.506986366388	1.378174189324	2.207815411941
H	3.836510813877	-0.205347137235	3.173879769585
H	2.323166789037	-1.481382512416	1.680567696279
C	2.148962243536	-1.333448979481	-1.020370260186
C	2.642027363632	-2.084965278155	-2.100558903887
C	1.775214181742	-2.802207850520	-2.923378475607
C	0.400298249048	-2.773442092827	-2.679860070518
C	-0.100663454797	-2.009624592861	-1.622815689630
C	0.758009827009	-1.281337874492	-0.792726310402
Bi	-0.056156309110	0.140430267086	0.794176743048
Cl	-0.465983903735	-1.664084444928	2.504318220698
C	-2.186138177334	0.059848324501	-0.025082443908
C	-3.101761853663	-0.937489581912	0.321379745076
C	-4.424034307869	-0.874845041987	-0.128666162018
C	-4.843271753691	0.201600484016	-0.914959970815

C	-3.942392346362	1.211272486106	-1.252918507230
C	-2.607589558138	1.143601057170	-0.822831349894
C	-1.639744830576	2.213286696352	-1.166058296374
C	-0.375174145649	1.881950629472	-1.692432864151
C	0.586901666372	2.869173236951	-1.927593541334
C	0.293983742102	4.206525563712	-1.661398212497
C	-0.968969365819	4.551144959518	-1.168761377948
C	-1.925911667823	3.566640597538	-0.923318675961
H	-2.898376389402	3.838251829634	-0.508797164859
H	-1.204471543763	5.596112879300	-0.959261528992
H	1.041926536737	4.979826561570	-1.841801017863
H	1.559469077690	2.587226235478	-2.333720361257
H	-0.170313080913	0.846012054209	-1.976527641654
H	-4.264420577432	2.049721238576	-1.874895930950
H	-5.874745184065	0.254542837426	-1.267154760012
H	-5.129960367413	-1.662113315556	0.143181665871
H	-2.781469814977	-1.763147688028	0.961669649274
H	-1.179762631366	-1.970009187447	-1.455649759182
H	-0.282747966112	-3.339729597041	-3.315880970130
H	2.174957991518	-3.390862852189	-3.751088267937
H	3.720073343550	-2.124385062385	-2.273071996508
H	4.100808710515	0.417957967260	-1.754538067916
H	5.641490860399	1.672478121947	-0.262729684822

Structure 3.

C	-1.871362684646	-2.884498224893	-0.272933883602
C	-1.504384646509	-1.561297678772	-0.525095626813
C	-2.477523086393	-0.554517769138	-0.652853332590
C	-3.830567976529	-0.913800695397	-0.543520519205
C	-4.196904822702	-2.235555441306	-0.289208682001

C	-3.219243533902	-3.224695028800	-0.148589224379
H	-3.509759133122	-4.256762800215	0.053085931658
H	-5.252527374964	-2.494680012504	-0.190182064472
H	-4.595372309046	-0.139606291638	-0.631508666053
C	-2.065002501857	0.849281563798	-0.882200275614
C	-2.619921871010	1.579701487563	-1.947022374208
C	-2.213597937520	2.888768930743	-2.197565765264
C	-1.251753436112	3.488593847323	-1.380670571358
C	-0.710066228339	2.776699339125	-0.308800645818
C	-1.114530056641	1.464531805753	-0.044025993121
Bi	-0.376761513987	0.390745681442	1.826514857218
Cl	-1.334287664208	2.099433130860	3.401533170464
C	1.622818139787	1.479342513530	1.661765797809
C	1.902500080490	2.661593603362	2.349776492445
C	3.083840536852	3.366981033780	2.098203215606
C	3.991216230830	2.892065277694	1.149310054686
C	3.728150270679	1.703188693084	0.468251361941
C	2.556350704235	0.979385896179	0.734790538561
C	2.298012818652	-0.306879816274	0.041909250995
C	2.288407597207	-0.401251753760	-1.359863993279
C	2.059942752602	-1.625249496019	-1.988707879130
C	1.838811466671	-2.779655198306	-1.230419932674
C	1.841973331238	-2.702126335705	0.162644474328
C	2.066943473664	-1.475555552391	0.793519598824
H	2.126045559048	-1.422835109062	1.883384626569
H	1.682217546839	-3.598887512064	0.763653676133
H	1.660861806499	-3.734588569718	-1.727165592665
H	2.045876039471	-1.679150364538	-3.078763709561
H	2.445827363514	0.501489549305	-1.952275764360
H	4.444666456346	1.315526753967	-0.259683857046



H	4.910039110954	3.443909502591	0.943997917633
H	3.289623314484	4.292622615657	2.638711290241
H	1.174540046906	3.054228432864	3.064950347371
H	0.023201163586	3.260488032396	0.340134169382
H	-0.926279619785	4.512045051795	-1.574819693624
H	-2.642167069481	3.439018428046	-3.036990413386
H	-3.354812411271	1.098469868316	-2.596157808186
H	-0.453322120252	-1.308741805320	-0.684407852095
H	-1.098632812278	-3.650461583351	-0.186786651361

Structure 4.

C	0.768801054899	-2.941824616345	1.665755610939
C	1.313136496450	-1.684347202266	1.386696058302
C	2.483509825316	-1.559466554181	0.611844248909
C	3.104316998866	-2.731584119168	0.148687322654
C	2.561841188385	-3.984684794187	0.431823486542
C	1.388926873353	-4.095227613061	1.185490344473
H	0.967771750989	-5.077432838631	1.403549349971
H	3.052580593746	-4.883357371387	0.055008042637
H	4.007613521509	-2.648839065320	-0.458393593456
C	3.013392521477	-0.216526256375	0.272732570269
C	4.369205947410	0.090559210912	0.471977249943
C	4.858042275569	1.358240209375	0.157468824849
C	4.000714018966	2.325460960699	-0.372975872630
C	2.654689731527	2.019302997737	-0.596034523996
C	2.150931035458	0.756327454959	-0.272622428181
Bi	0.027881566068	0.101907454255	-0.801530030967
Cl	-0.448039694919	2.132453709769	-2.201244570893
C	-0.908383893152	1.045660328122	1.053009116674
C	-0.175304215803	1.913367309495	1.869106036825

C	-0.781215930471	2.566985144208	2.945119001620
C	-2.136095185638	2.356881735668	3.209599049365
C	-2.875550092232	1.489978679379	2.405940259579
C	-2.270333899072	0.813913057267	1.333062205296
C	-3.073342578699	-0.114907554192	0.500476811709
C	-4.259052176044	0.313280705918	-0.116930966984
C	-4.995972305563	-0.554420834527	-0.922870245897
C	-4.564810975225	-1.868443178883	-1.122991787016
C	-3.394945671191	-2.312707430430	-0.504631882966
C	-2.657024918570	-1.443308849404	0.300745773440
H	-1.763363210467	-1.805796023412	0.814358468240
H	-3.057504899494	-3.341276107923	-0.642280817111
H	-5.141439121279	-2.544306162859	-1.756355365168
H	-5.907914975525	-0.199893472818	-1.405462244413
H	-4.583821185213	1.346014739020	0.019219211415
H	-3.931514882168	1.310328100409	2.619380059848
H	-2.617471054790	2.864160874249	4.047388769785
H	-0.196564537860	3.243180165801	3.571941569528
H	0.878301500517	2.103449886977	1.651235150145
H	1.991882645890	2.765392366312	-1.041464523522
H	4.382306153521	3.316843847750	-0.623986482934
H	5.910048516511	1.592127112322	0.329296749332
H	5.033599273420	-0.664357845897	0.898584651328
H	0.863754452160	-0.789844126997	1.825881526008
H	-0.129562538633	-3.017039032336	2.281327816509

## **R<sub>2</sub>BiBr**

Structure 1.

C	3.180375791267	-1.577826114151	-0.213692552058
C	1.880056819753	-2.094196534907	-0.185327854985

C	1.073457058852	-2.087289965646	-1.341371143082
C	1.621808783360	-1.590587525518	-2.533725491390
C	2.919230712122	-1.082102451521	-2.562413431691
C	3.699205771108	-1.065013680772	-1.401940391117
H	4.710732550750	-0.658309184420	-1.426818749327
H	3.317866952910	-0.675767939342	-3.493190109896
H	0.999842465833	-1.558462069809	-3.429511346634
C	-0.345844808792	-2.509789195116	-1.268171210285
C	-0.867958337107	-3.468863131110	-2.148120037062
C	-2.212794416182	-3.833221761102	-2.071549137372
C	-3.047638826341	-3.229375472171	-1.128740565647
C	-2.537715384589	-2.253364642020	-0.266307435484
C	-1.192747778414	-1.883548856849	-0.331041135151
Bi	-0.253697241541	-0.240033237755	0.957636852104
Br	-2.599997678257	0.839184840292	1.670483111974
C	0.065677701882	1.066919230639	-0.878820780316
C	-0.723287377330	0.902041002051	-2.020707123561
C	-0.427001032818	1.589931868396	-3.198915264449
C	0.676447294410	2.445828299789	-3.243180301640
C	1.457595949325	2.632282946318	-2.104508276851
C	1.149960234138	1.965030804668	-0.905632948185
C	1.964224089284	2.216175397680	0.306903924638
C	3.366333724865	2.146367081072	0.271376452111
C	4.120811567942	2.355576520607	1.425622203646
C	3.488131089686	2.646150676533	2.637877770752
C	2.095851010887	2.737525161305	2.684673967069
C	1.340456904787	2.528576582570	1.528955663692
H	0.253487379932	2.649801487003	1.558958490278
H	1.592593511973	2.985160116696	3.620669818911
H	4.079505101380	2.808096623075	3.540326857152

H	5.209541857269	2.285138158879	1.381558435091
H	3.859664279094	1.894042463196	-0.668577872530
H	2.301332582442	3.325758665146	-2.125194656863
H	0.919618573242	2.981657460334	-4.162301751325
H	-1.053239113234	1.453311308186	-4.082877859561
H	-1.566977808740	0.208640891900	-2.001930842685
H	-3.203520727549	-1.753480287877	0.441959063572
H	-4.100488336201	-3.511843856274	-1.069403956001
H	-2.609449323580	-4.591459760017	-2.749203918620
H	-0.209085659715	-3.940442299412	-2.880963742688
H	1.501446879713	-2.568390717607	0.724448473887
H	3.787401212187	-1.587468902936	0.692817801581

Structure 2.

C	0.581329875162	4.521026982603	1.388095140419
C	1.629272396635	3.651977781698	1.083820246115
C	1.455716197527	2.620428159143	0.146603038009
C	0.208204812733	2.510482109724	-0.501322953925
C	-0.845930227723	3.373984986268	-0.184010978749
C	-0.663720297063	4.377892132099	0.766630067980
H	-1.483706902768	5.051245452277	1.020272728584
H	-1.805031220707	3.261476978807	-0.692418680678
H	0.083533107250	1.778979409979	-1.304846063577
C	2.522863032078	1.623542185537	-0.111624914308
C	3.834089573608	2.031499740631	-0.404530366425
C	4.832340698366	1.084914720321	-0.631674093096
C	4.534807890031	-0.277232584490	-0.547427624584
C	3.236104766294	-0.689904910489	-0.234097516624
C	2.222785338068	0.248398053619	-0.021712987007
Bi	0.103425571107	-0.292615706428	0.643794992069

Br	0.668838030423	-2.864036036961	1.151013900166
C	-0.594383768316	-0.708751463241	-1.489284830583
C	0.327906243517	-0.945412843037	-2.513663117316
C	-0.093392241760	-1.083588788063	-3.838445454962
C	-1.450283808333	-0.971332399756	-4.149866957575
C	-2.378625734058	-0.735311819839	-3.137531537124
C	-1.966611169594	-0.615934251035	-1.799114637604
C	-2.971463845368	-0.377759379020	-0.734668554999
C	-3.892738648345	0.677570644748	-0.831921467515
C	-4.809734309247	0.920429189376	0.191352191769
C	-4.827152914340	0.107361507010	1.327969854616
C	-3.929328454851	-0.957130590422	1.429188396162
C	-3.009678248366	-1.199659424690	0.406704477201
H	-2.335451500808	-2.058406073833	0.472682515615
H	-3.946801655375	-1.609075598667	2.304317551346
H	-5.543243723363	0.299613637739	2.128676789977
H	-5.510391953987	1.752984275302	0.104374272996
H	-3.870685415564	1.322419539074	-1.713275140092
H	-3.442668771380	-0.667840202671	-3.375409745592
H	-1.787752612560	-1.075132186915	-5.182490072634
H	0.638094263444	-1.273372041690	-4.626121491490
H	1.393232233668	-1.009812484699	-2.281468019102
H	3.013998478411	-1.756174187543	-0.138069745434
H	5.316186404517	-1.020349084011	-0.717934836073
H	5.844644181675	1.411670753036	-0.875127222332
H	4.060439912810	3.097707027007	-0.478466290397
H	2.587062416657	3.745974858175	1.598525588253
H	0.731690999895	5.307425933327	2.130107548521

Structure 3.

C	1.492774856358	3.021989237528	-1.069672721643
C	1.797260071344	1.657618664192	-1.023569952957
C	2.858515764998	1.180390496734	-0.228556102777
C	3.622425487489	2.113250484711	0.491853290784
C	3.320225392751	3.473879855524	0.440162119958
C	2.249537109111	3.933375965442	-0.333375927088
H	2.014800724249	4.998343237053	-0.368052654680
H	3.918279161645	4.181518031562	1.016787642428
H	4.443352639592	1.757170863795	1.117295862727
C	3.118533861195	-0.276155517760	-0.131020604768
C	4.412879766025	-0.787175049565	-0.319007927283
C	4.647686845156	-2.158914552072	-0.233854562255
C	3.595127777347	-3.030193251873	0.056480497904
C	2.308657832833	-2.525561796538	0.268358257044
C	2.057440973520	-1.153773188448	0.172154998590
Bi	0.038671952974	-0.213109573314	0.683585354303
Br	-0.985798040798	-2.427239244441	1.783576959743
C	-0.864655967039	-0.685803742554	-1.355114763494
C	-0.200650011255	-1.507634215567	-2.271507516406
C	-0.808925755918	-1.875370157598	-3.473950109394
C	-2.097255523651	-1.423434269648	-3.766386748564
C	-2.766107812096	-0.597639126582	-2.863863391602
C	-2.154398325912	-0.207210004927	-1.661473724731
C	-2.877167159011	0.685644705098	-0.722849048065
C	-4.148345032100	0.344869828575	-0.235298313425
C	-4.807305202537	1.173065624277	0.673290531345
C	-4.210464471909	2.359883329641	1.106688468865
C	-2.952077419368	2.718363090338	0.620450854989
C	-2.291869469506	1.887860879422	-0.286885176646

H	-1.324039654727	2.188454448305	-0.695195756104
H	-2.483977720638	3.649770007220	0.942634797961
H	-4.726651290450	3.004771675475	1.819553918649
H	-5.787925777738	0.885186657794	1.054401985207
H	-4.602651806179	-0.594554739903	-0.553861889842
H	-3.766902940264	-0.227404617435	-3.094869517455
H	-2.580236474385	-1.709822946062	-4.702027598605
H	-0.279109578825	-2.519504642225	-4.178467463617
H	0.795704548825	-1.888572965301	-2.037289140524
H	1.493833783378	-3.206743777680	0.526938827776
H	3.777353673172	-4.104406785104	0.128488544225
H	5.653905624023	-2.548722740601	-0.396602472538
H	5.229882038742	-0.103237608258	-0.558917575978
H	1.248469286620	0.957483493426	-1.660046659200
H	0.675104262958	3.372179937344	-1.703006592854

Structure 4.

C	2.058062220893	-3.456281345355	-1.079048517203
C	0.836733435263	-2.834619094735	-1.334418579240
C	0.787414204995	-1.488800011294	-1.732313624205
C	1.991829251231	-0.787823973198	-1.887382959522
C	3.214473292957	-1.412378226040	-1.641073024337
C	3.251706133845	-2.746646373808	-1.233496087016
H	4.207648499644	-3.232842279374	-1.032046226827
H	4.140334049171	-0.848408359948	-1.764178753380
H	1.966437970743	0.252333964343	-2.209880309232
C	-0.505037681722	-0.827694909903	-2.030823989467
C	-1.358783929022	-1.422089321796	-2.976075271159
C	-2.567902201426	-0.829019675911	-3.339408306957
C	-2.948846191940	0.381055866156	-2.761993578428

C	-2.117003234625	0.971254387210	-1.807738297049
C	-0.907717984518	0.377816412943	-1.420002812019
Bi	-0.082252961270	1.423849699327	0.430271309801
Br	2.366945756092	2.308694129981	-0.222136685200
C	0.617501017655	-0.489750715882	1.446753353737
C	1.954315363459	-0.793535801360	1.704200312427
C	2.297290202678	-2.015195428584	2.290542460471
C	1.303132021396	-2.939819586353	2.615825420815
C	-0.036018425002	-2.643050276232	2.362541629081
C	-0.389302477618	-1.411035766853	1.794620631919
C	-1.804932176009	-1.071321682104	1.510336502653
C	-2.364121892960	0.113310993459	2.029204592739
C	-3.664892258849	0.502155989905	1.689891155957
C	-4.427436214043	-0.291606492074	0.834619789177
C	-3.891809794836	-1.482913209455	0.334541340183
C	-2.596632775425	-1.870922319771	0.671283490946
H	-2.170229545855	-2.782564432130	0.251226045164
H	-4.482163953998	-2.103500042421	-0.341421990005
H	-5.438557893657	0.011309672925	0.560582611006
H	-4.082167073011	1.419902254826	2.106922723631
H	-1.790161044597	0.697875341192	2.753448079262
H	-0.819363815677	-3.358836278848	2.621130159174
H	1.571538123411	-3.895843693352	3.068306705882
H	3.346263194867	-2.250200131226	2.480048088340
H	2.737065897364	-0.089384220191	1.412218130992
H	-2.443146175440	1.904933901046	-1.336623392626
H	-3.886684706444	0.861179145132	-3.045937284243
H	-3.204668692257	-1.307955696737	-4.085552641267
H	-1.044982159804	-2.354972891565	-3.448756638768
H	-0.094642754516	-3.388752943112	-1.201629503041



H	2.077474378856	-4.495335578832	-0.746879062166
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## **R<sub>2</sub>BiI**

Structure 1.

C	-2.413168587520	3.409443335570	-0.204502383246
C	-1.020580750985	3.396808752084	-0.266709168371
C	-0.265685057260	2.765889490603	0.733813200998
C	-0.947835783297	2.178488671775	1.818684949578
C	-2.346049056016	2.186586051786	1.877125720575
C	-3.080117642888	2.797291735820	0.861313400075
H	-4.170721287917	2.801437146764	0.901102161030
H	-2.856814857237	1.723583844718	2.722721924993
H	-0.369362948198	1.770814387388	2.652592099257
C	1.206812483714	2.633833657124	0.617480985481
C	2.024163991792	3.756744709692	0.422939099073
C	3.405052457124	3.606911377159	0.290197149358
C	3.975525650105	2.332999207269	0.336344514601
C	3.162447604825	1.208086377365	0.509835874077
C	1.779522376763	1.345349636189	0.644724447888
Bi	0.310734657010	-0.406451656408	0.825482071353
C	-0.540365509617	0.090990921365	-1.227487629053
C	0.220274351281	0.792414341238	-2.167426094865
C	-0.354099052833	1.244670643088	-3.356842903534
C	-1.707375749437	1.005450363012	-3.608674654211
C	-2.468878748970	0.289110907426	-2.687811687083
C	-1.891913378312	-0.196110480913	-1.500862891679
C	-2.707545242309	-1.004347994617	-0.563865648257
C	-3.970829432388	-0.569955526826	-0.131278914720
C	-4.717618422464	-1.331493237060	0.767154017878
C	-4.218203058976	-2.545691872102	1.247246252625

C	-2.970844861404	-2.998163660659	0.813336114131
C	-2.222453943137	-2.235928560349	-0.086331434595
H	-1.267331906503	-2.618265611119	-0.457337755388
H	-2.580026212227	-3.953871025435	1.165155211141
H	-4.803846367838	-3.140429885426	1.950143898366
H	-5.693096784179	-0.973717027863	1.100384765398
H	-4.351097001693	0.388688630736	-0.486546313041
H	-3.518111471900	0.069862924084	-2.896152481841
H	-2.165987926256	1.363535240844	-4.531944956403
H	0.253134929328	1.787723651006	-4.083858275530
H	1.269525140899	1.013174955185	-1.960510124059
I	2.167663366451	-2.427145493184	-0.097424384505
H	3.609918674168	0.210515796799	0.503002102053
H	5.055257864149	2.211459140089	0.227318262552
H	4.035676253377	4.486285644755	0.149282107925
H	1.571464032980	4.750445011223	0.391116502501
H	-0.504301696542	3.833514129238	-1.122533272973
H	-2.983942095662	3.882622350568	-1.005231859553

Structure 2.

C	4.995020666256	-0.052378734179	-0.344651795237
C	4.093277023935	0.035037259217	0.716139023175
C	2.952113338635	0.848283822327	0.623126876843
C	2.751452663113	1.590882500968	-0.554466886250
C	3.654763024492	1.503329541666	-1.615563472038
C	4.775558211277	0.676865723677	-1.516477249805
H	5.480507237857	0.605703769458	-2.346576893136
H	3.483662955637	2.091125583515	-2.519007890696
H	1.895737079809	2.269426286872	-0.620492841494
C	1.968357061606	0.914106143950	1.730540486095

C	2.406902503047	1.186614568639	3.038036580290
C	1.499368003931	1.261279256747	4.093013655530
C	0.138584194375	1.055036506518	3.856598365587
C	-0.304786470912	0.765572633192	2.564041632194
C	0.596338583355	0.689063954835	1.497677266736
Bi	-0.092604348435	0.030168632251	-0.576402459684
C	-2.001495439595	-0.956749520328	0.216160465827
C	-3.198048296061	-0.278352709152	0.461467388596
C	-4.348224206173	-0.976099081733	0.842282324158
C	-4.312900233380	-2.367287664822	0.962225248352
C	-3.129205373654	-3.058139910835	0.705068638078
C	-1.964798751968	-2.361610921401	0.343726033364
C	-0.702496168475	-3.086203879236	0.059211367061
C	0.504448009238	-2.670080449323	0.657362144735
C	1.720769948784	-3.270331752191	0.315431431759
C	1.747481869233	-4.314052702175	-0.608757818735
C	0.551850441652	-4.760624637066	-1.180805524121
C	-0.660112601545	-4.153314576445	-0.852839245159
H	-1.585109920769	-4.482080005291	-1.330014071465
H	0.566726749168	-5.579940542165	-1.901946911555
H	2.693436816893	-4.784016756505	-0.880160637700
H	2.642668401699	-2.924562980498	0.784846218639
H	0.477201892581	-1.906562695626	1.439828762329
H	-3.093497355236	-4.145311964881	0.807725072783
H	-5.209220078539	-2.915808136336	1.256809598958
H	-5.274920056617	-0.432583937381	1.036934615274
H	-3.239578801348	0.807118680757	0.335214235643
I	-1.318852910194	2.576450246936	-1.206559443867
H	-1.367486700053	0.582349474466	2.391198124718
H	-0.577864394861	1.115513554216	4.677971321045

H	1.854357143804	1.488186552499	5.099692374160
H	3.469370457560	1.367828209615	3.215196869476
H	4.258762179089	-0.545829625836	1.625977011518
H	5.871305650790	-0.697608718919	-0.259179991982

Structure 3.

C	3.437403224457	-1.547511158949	-1.406517397710
C	2.484985945210	-1.400809158351	-0.396411015200
C	2.734558555710	-0.578566334434	0.716303738555
C	3.972485791992	0.078363234153	0.800131817639
C	4.923703672776	-0.067128815872	-0.210176350363
C	4.658467794597	-0.876652861617	-1.318653016442
H	5.404431345710	-0.987609102457	-2.107482450973
H	5.875477411822	0.461550221664	-0.136728887153
H	4.173646621837	0.726611793120	1.655043069677
C	1.697146558352	-0.414304081739	1.760743492819
C	2.019681665258	-0.640610827385	3.109599579328
C	1.046984405702	-0.527921875839	4.100831682327
C	-0.260399128994	-0.175751927392	3.757050538544
C	-0.584931737438	0.069017733104	2.421429217899
C	0.383347586796	-0.039217797069	1.418554838167
Bi	-0.110226299753	0.518700254241	-0.738413055897
C	-2.301326670216	-0.017064383858	-0.349970050071
C	-3.305934502241	0.907897559602	-0.058376742038
C	-4.581026537097	0.475259802883	0.321479410170
C	-4.854578903981	-0.890229680319	0.419544894719
C	-3.861795657121	-1.822751122467	0.116099297926
C	-2.589357187795	-1.394314367891	-0.290860894178
C	-1.543381262215	-2.382717779743	-0.656455973059
C	-1.108620527245	-3.367319139747	0.246367570671

C	-0.121722992428	-4.281873516797	-0.120790611105
C	0.445484715979	-4.236606998666	-1.398912979308
C	0.023853968945	-3.265529598146	-2.308010812856
C	-0.958096067963	-2.341641313910	-1.937468427813
H	-1.324145570365	-1.610703414514	-2.662194856356
H	0.452485086861	-3.227654394108	-3.310629213225
H	1.218160681555	-4.953918007030	-1.679570936613
H	0.216419687238	-5.029593756995	0.598382962275
H	-1.536581276722	-3.391103412733	1.249500891922
H	-4.074698171187	-2.892816511158	0.171834600867
H	-5.844374743110	-1.232210517493	0.726176330964
H	-5.357786715643	1.207439045372	0.550487771553
H	-3.081944371337	1.977897614524	-0.091282322574
I	-0.422489223252	3.337859985633	-0.173950986245
H	-1.603283912240	0.366538588599	2.163622828154
H	-1.026958458133	-0.085143711250	4.528983504858
H	1.308287438847	-0.721489681473	5.142763088990
H	3.037982942051	-0.936671955846	3.370361938815
H	1.555844087144	-1.973545142835	-0.436664875883
H	3.226214727637	-2.198338484813	-2.257258211776

Structure 4.

C	-2.821763862894	-2.897179341448	1.002113499188
C	-2.149353617705	-2.270406566037	-0.048810224426
C	-2.733484841097	-1.193539286424	-0.739361338307
C	-4.015833762224	-0.769812268226	-0.356886253617
C	-4.687019990850	-1.394390568406	0.694544370809
C	-4.091367319721	-2.456725027510	1.379698043327
H	-4.616863488674	-2.940598118720	2.204164516702

H	-5.676300817890	-1.041824049813	0.989112777053
H	-4.470262216549	0.077098949432	-0.873420510470
C	-1.995816221108	-0.513304677226	-1.831507674689
C	-2.573998077752	-0.402337684169	-3.106190610271
C	-1.884287154418	0.217204539937	-4.147805373837
C	-0.610131786302	0.742514787198	-3.924516522309
C	-0.037589709441	0.657165908306	-2.653098918598
C	-0.720915183247	0.040917597788	-1.600259531705
Bi	0.117779348266	0.027193897677	0.521015039664
C	2.123974828261	0.937208241126	-0.108413610426
C	2.334150667879	2.303481290008	-0.312657436047
C	3.615975520749	2.793339657104	-0.579356743250
C	4.704020227370	1.918219012189	-0.619461755098
C	4.509597010476	0.554420205318	-0.403901281130
C	3.220408308636	0.052212199106	-0.164167602905
C	2.996740497402	-1.397272484694	0.054090742592
C	2.000604403680	-2.076993965188	-0.675360656464
C	1.719474586054	-3.423588880254	-0.421024894869
C	2.434663242966	-4.115725100270	0.556609785107
C	3.442425572955	-3.457596882170	1.269070657743
C	3.722394274564	-2.114169424210	1.019624872678
H	4.490241108248	-1.597230113375	1.598242961672
H	4.006386900219	-3.993409164289	2.034569809870
H	2.215904557307	-5.165140022860	0.758673490914
H	0.952616379102	-3.934994491805	-1.006192362493
H	1.481474007168	-1.556984546467	-1.485599704770
H	5.355580076172	-0.135314479144	-0.447566228571
H	5.706605473622	2.298444566711	-0.822431125330
H	3.766778218018	3.861912644867	-0.746100822228
H	1.490371490478	2.995647791926	-0.245335416035

I	-1.169602062863	2.535860831716	1.165226369607
H	0.946364653912	1.097562659816	-2.477474754829
H	-0.064608669475	1.226238157425	-4.736810337428
H	-2.341119623361	0.285612635879	-5.136744624700
H	-3.564616715102	-0.827282775711	-3.279715658021
H	-1.172265555703	-2.640719966613	-0.367364153679
H	-2.353431677127	-3.734166688502	1.522469189574

Optimized structures from crystal geometries

### **R<sub>2</sub>BiCH<sub>3</sub>**

C	1.158713064007	2.176117831170	4.668741074662
C	-0.113578944621	2.208892411057	4.085529950155
C	1.371947916557	2.880537327446	5.873721281666
Bi	2.927495947426	1.179798581239	3.618857701950
C	-1.165981311894	2.915688238072	4.674221143846
C	0.312874511059	3.599384336920	6.453992766781
C	2.701301326162	2.890876597093	6.534323911282
C	1.705684008672	0.585239938675	1.768708155325
C	2.520124197448	-0.870813940646	4.551013561946
C	-0.949796647154	3.613856248896	5.863245727231
C	3.370518210966	1.689402186639	6.826793108238
C	3.325560075867	4.102048065115	6.875351131463
C	1.321857016937	-1.117830767857	5.230597760397
C	3.437972515635	-1.926109888925	4.378371430704
C	4.632051505348	1.700714085772	7.425815036163
C	4.586286400266	4.112878839285	7.472731444850
C	1.018022543830	-2.390674997930	5.721227770044
C	3.117265143278	-3.208300039877	4.856887493730

C	4.732752892966	-1.712446489962	3.684191154899
C	5.246952684787	2.912235299855	7.746413848994
C	1.917949453249	-3.440317379544	5.528853994412
C	5.628759304343	-0.723524243018	4.126935821547
C	5.094009821251	-2.490655270427	2.573175393812
C	6.842106728403	-0.511292470025	3.470986910051
C	6.304288021591	-2.274992698213	1.912931260236
C	7.181317357275	-1.282957716060	2.358023153486
H	2.821109746750	5.042675651066	6.646352062282
H	5.128207020696	0.755760077929	7.654882509057
H	5.059348273769	5.064909713606	7.718985118479
H	6.232943631335	2.922195882959	8.212802975403
H	2.880326389385	0.737455973297	6.612814354139
H	0.482123324613	4.129759516251	7.393530537360
H	-1.764955146854	4.166502260492	6.333401146242
H	-2.150633191560	2.922905499505	4.202342840935
H	-0.295681635299	1.678426497395	3.148848881165
H	1.386775525965	1.485969648227	1.229786184500
H	0.838481364744	-0.009629526815	2.077360751246
H	2.356371460400	-0.021683138748	1.125409115659
H	0.601124748377	-0.307805212604	5.367978591666
H	0.077836911278	-2.560910625749	6.249394978812
H	3.833832393645	-4.020992481524	4.717636368638
H	1.690739944347	-4.437873562912	5.908330257162
H	4.403173396594	-3.257236813275	2.215796191100
H	6.560960430138	-2.881401404659	1.042635404951
H	8.127409642640	-1.115644504002	1.841256465221
H	7.526543573002	0.256966154514	3.835051705231
H	5.380668452382	-0.136103689704	5.013941572883



**R<sub>2</sub>BiCl**

C	8.495459010714	2.661717858951	8.052245545053
C	8.010072398215	3.919024960642	7.679810210535
C	8.892457172135	1.735167384406	7.085950209378
Bi	7.540535613694	5.488630897379	9.269554587731
C	7.905310222077	4.247040025084	6.314341494114
C	8.808694896760	2.065895492402	5.731026098826
Cl	9.901993472987	5.600666366540	10.121436019468
C	6.961954253106	3.826296231058	10.723603772299
C	8.322968925315	3.314996648736	5.348601031227
C	7.361278034480	5.558477852028	5.893856026163
C	7.833423671111	3.322250016663	11.690697057209
C	5.705087064116	3.221983847007	10.537765659095
C	8.065624137408	6.397546277432	5.015858898215
C	6.119437215719	5.995183289785	6.388105380845
C	7.475660975554	2.206056628489	12.453768478080
C	5.361430566698	2.087247233220	11.286888746378
C	4.754171275202	3.785165865692	9.547583869460
C	7.553145180579	7.646124151358	4.663431548477
C	5.606095525840	7.244211290302	6.034254450189
C	6.244070257718	1.582914344109	12.242979801171
C	4.251671471944	3.013012030669	8.487169680094
C	4.329501244675	5.123073162749	9.663610203492
C	6.324785716413	8.076166452870	5.174355665994
C	3.348170287668	3.559989323880	7.576146161393
C	3.417135663550	5.667360621824	8.755267485902
C	2.924527824143	4.886290428112	7.709652196932
H	8.814969362586	3.783428774042	11.824421467411
H	9.034933059803	6.073769634390	4.633211816297
H	5.529310733614	5.318881886641	7.011018334039

H	8.120598794911	8.293570671457	3.992440152531
H	4.636045412057	7.556232443395	6.423878159497
H	5.930105246152	9.054605902286	4.897902987882
H	8.583498556845	2.405818992654	9.110421475926
H	9.271275727477	0.758311301919	7.391589255918
H	9.116231051523	1.346509140260	4.970075998902
H	8.237141071928	3.570746365287	4.289995454848
H	4.593223510875	1.982897986542	8.373419352801
H	4.677920671933	5.716109039425	10.512740612160
H	2.975485687424	2.950606665233	6.751247392119
H	3.085531527708	6.699935305119	8.873724124844
H	2.215246961804	5.308313205436	6.995951369217
H	8.164840898643	1.817190419923	13.206011839255
H	4.389106445496	1.614460533886	11.131285336142
H	5.966003201397	0.704863050716	12.828304592491

### **R<sub>2</sub>BiBr**

C	-0.972303825116	-2.021728107663	9.233738529519
C	-0.285764184705	-2.386226974589	8.071718718779
C	-1.977633278214	-2.871908408907	9.737509822507
Bi	-0.628692956484	0.008474671915	10.213580124828
C	-0.586036767274	-3.574958549034	7.403635565665
C	-2.289331090794	-4.055301773950	9.047108739364
C	-2.716221268826	-2.522397592631	10.974646599795
C	0.331293560910	0.891864048961	8.335624387138
Br	1.694574223163	-0.703231842393	11.343247050589
C	-1.596198793053	-4.407296308067	7.890500161761
C	-2.016576521082	-2.197836748204	12.151415112779
C	-4.119807725324	-2.486429430160	10.997674292174

C	1.682702786646	0.743031124785	8.012427059577
C	-0.486606217838	1.713096029240	7.531562538447
C	-2.702697486139	-1.829522243460	13.310480835935
C	-4.804472384241	-2.116476907949	12.155852796165
C	2.221789407235	1.383022568177	6.892395082422
C	0.067320337256	2.372531532900	6.422518280480
C	-1.914400974887	1.894448704945	7.888815043144
C	-4.098043834692	-1.781636274518	13.314407703068
C	1.412383629218	2.198712326784	6.098304209033
C	-2.477667692259	3.173501717832	8.027355528802
C	-2.727366893339	0.774484277586	8.157548868268
C	-3.797351020389	3.327730361568	8.451611410630
C	-4.046269222446	0.931494579806	8.596420161204
C	-4.583006541457	2.209553712063	8.749414056439
H	2.326517668668	0.130518951301	8.649352018236
H	-0.925311379312	-2.272585346058	12.163681828406
H	-4.673085202502	-2.733458546761	10.089042223158
H	-2.141934558151	-1.586292834418	14.214483268827
H	-5.895715460205	-2.082756947917	12.152856642117
H	-4.634520273324	-1.490304778586	14.218655408476
H	-3.066811051511	-4.713019298825	9.442281077536
H	-1.840690653179	-5.335949752445	7.372266182799
H	0.485752114032	-1.727226700682	7.667512278223
H	-0.037259900265	-3.846189524299	6.500103671130
H	-1.859411648364	4.050670571287	7.828100319071
H	-2.338950091188	-0.228084058396	7.958774272091
H	-4.212778581073	4.330400407369	8.566896458670
H	-4.652375955702	0.048745490189	8.806014987604
H	-5.609928297700	2.337347619616	9.093673720457
H	-0.571432651175	3.001719517581	5.798335818247

H	1.829332626443	2.700045276552	5.223309318717
H	3.276978028640	1.251045459457	6.645277827724

**R<sub>2</sub>BiI**

C	1.223401754709	2.283655427261	2.175777442652
C	1.168493380691	3.188778701365	1.113926343895
H	1.940227195734	3.958190316516	1.017546443596
C	0.160839663147	3.091536620177	0.148692496187
C	-0.796935784172	2.079714104811	0.238553437974
C	-0.758812325815	1.178024179571	1.302711048922
C	0.235374046075	1.286463548289	2.285957124681
C	0.250067271104	0.350360644514	3.438443627745
C	0.340679628247	-1.039484623027	3.255357229979
C	0.340075512547	-1.902882709515	4.350410669894
C	0.245603861500	-1.395355708920	5.650682576548
C	0.159936606999	-0.016879034700	5.849749164480
C	0.166419602773	0.849913319064	4.752793567705
C	3.827324371166	0.415849121205	2.542482402745
C	3.626182032934	0.289704367222	1.164690582103
C	4.271335575403	-0.714029829104	0.439253828046
C	5.136495745171	-1.596633239356	1.091138650469
C	5.340544259690	-1.482134612378	2.465050390781
C	4.675637241303	-0.490995903383	3.207228123057
C	4.862282175414	-0.413304268816	4.674791285501
C	3.740485882030	-0.409662340084	5.522308856683
C	3.888231604022	-0.309033053282	6.906384692942
C	5.163081692958	-0.213951520927	7.467268607212
C	6.286604219952	-0.230636732691	6.635817762244
C	6.139102659531	-0.333027884539	5.252355616672
Bi	2.921121586250	2.158927407965	3.703284421950

I	4.583682762120	4.152800158041	2.430757666903
H	5.283751968866	-0.132109237276	8.548866875689
H	2.746984842447	-0.541830735294	5.089154430582
H	3.003055441023	-0.316974253283	7.544548680449
H	7.285523153198	-0.153288532211	7.068489434850
H	7.017187137109	-0.322791823372	4.604042393786
H	2.975570961778	0.994437499622	0.642742722240
H	4.104892119252	-0.800791048489	-0.636455427591
H	5.647694695628	-2.380445861707	0.529359590618
H	5.998156715856	-2.183194229931	2.983660020323
H	0.130264025089	3.803427678441	-0.678866456223
H	-1.579921830152	1.995215082627	-0.517518680936
H	-1.515987365557	0.395318178383	1.389905664698
H	0.433701486430	-1.434509782609	2.242236446638
H	0.045038032961	1.925560034862	4.903179349529
H	0.423235318175	-2.979318576318	4.190202845615
H	0.244885702183	-2.073859356821	6.504726162260
H	0.075655374231	0.388278508097	6.859431885905

Selected geometries from potential energy surface of aryl ring rotation of R<sub>2</sub>BiBr

R<sub>2</sub>BiBr (a)

1.

C	3.226693579177	-1.613719890331	-0.244012673916
C	1.917306751898	-2.123559333902	-0.208336359914
C	1.085132486437	-2.067162643098	-1.352594630876
C	1.613840966819	-1.520360869203	-2.541410291371
C	2.920844195801	-1.016869276611	-2.577292720354
C	3.728720578140	-1.055325695492	-1.428180791557
H	4.753006683538	-0.654147246593	-1.458112057843
H	3.306555628189	-0.572261454711	-3.507116020251

H	0.969529116440	-1.449836089997	-3.429987225953
C	-0.338943342751	-2.492017831779	-1.275140405296
C	-0.871747739607	-3.423053585432	-2.192166895920
C	-2.222533847393	-3.794551257717	-2.124960255819
C	-3.059466151461	-3.227872562534	-1.150806196737
C	-2.545365559757	-2.281439884279	-0.246956178375
C	-1.192360208049	-1.912793332006	-0.302500191689
Bi	-0.310218510542	-0.244440814034	1.028715739552
Br	-2.701019044413	0.794138320284	1.674989780255
C	0.026064225538	1.064203349573	-0.831749682162
C	-0.769858902489	0.876330053003	-1.974119169394
C	-0.447616473085	1.518696988929	-3.179766909399
C	0.688700987972	2.341093723135	-3.249904250503
C	1.476019874441	2.545626968863	-2.109647211015
C	1.146752428022	1.928920154678	-0.880024039269
C	1.965177820498	2.210004480034	0.329935712913
C	3.372896747235	2.103777084220	0.302029855894
C	4.133548846863	2.350394150080	1.453690817286
C	3.502150359822	2.713513497767	2.654841874275
C	2.104814518458	2.840150336947	2.693238150432
C	1.342668648445	2.595403504567	1.540644915229
H	0.249895730508	2.737858947758	1.564050929131
H	1.601735442302	3.143755092354	3.623867658304
H	4.100253511407	2.904598411681	3.558681126911
H	5.229366547935	2.251440297107	1.415795142058
H	3.865693701506	1.796903090256	-0.632325650891
H	2.346214116885	3.219139785643	-2.152829522297
H	0.954024367161	2.839932425394	-4.194661169938
H	-1.080339826480	1.368681099727	-4.068335954018
H	-1.641732926712	0.204881588134	-1.931372916582

H	-3.213436531126	-1.801669102476	0.487388061346
H	-4.121825609336	-3.512960230241	-1.100663473216
H	-2.623713511430	-4.530589009004	-2.838362599714
H	-0.210556217845	-3.867657420677	-2.952633551825
H	1.546327413370	-2.621347501919	0.702360805334
H	3.858013127668	-1.663448318098	0.655867427174

2.

C	3.402082908621	-2.816127699088	-0.105573713984
C	2.039145444712	-3.114733807102	-0.253685722458
C	1.231148397717	-2.369020522807	-1.141518293817
C	1.826782867744	-1.326991235343	-1.889255349861
C	3.190122883554	-1.028513508569	-1.735531077260
C	3.979112023335	-1.768368358358	-0.841617741755
H	5.045845191211	-1.528333609605	-0.716867897270
H	3.634666683070	-0.209133102967	-2.320465655179
H	1.208562397501	-0.743001297153	-2.586359385283
C	-0.240272530959	-2.631757094287	-1.240730790309
C	-0.755068791323	-3.669632915579	-2.042967859433
C	-2.139963501528	-3.891402743784	-2.108350567265
C	-3.019626745593	-3.083954046964	-1.370046215154
C	-2.515447472170	-2.050278253500	-0.561061310786
C	-1.132178588578	-1.822290021898	-0.498390806623
Bi	-0.125903812340	-0.207787936484	0.790467985652
Br	-2.414837905877	0.727309336107	1.823366119322
C	-0.083856869100	1.268239430895	-0.974609887178
C	-0.949066927216	1.091640156523	-2.068051551592
C	-0.797143641264	1.866348424086	-3.229250778691
C	0.237021739113	2.813602851425	-3.305751199563
C	1.096642113034	3.001424156304	-2.215238136969

C	0.940165099058	2.246028685421	-1.030312356486
C	1.847005996114	2.483417513162	0.125014012765
C	3.249741146621	2.466663778983	-0.034629138190
C	4.098368291145	2.658978334732	1.064968343066
C	3.560265308699	2.877924432245	2.343650786227
C	2.167403233094	2.911801129092	2.514494010599
C	1.316808796044	2.719294098083	1.415259653104
H	0.224250158299	2.780178042764	1.547713908590
H	1.736007534687	3.098650565342	3.509629329970
H	4.227266437657	3.026561418972	3.206278776925
H	5.189728905943	2.630258436186	0.923988018299
H	3.673103682532	2.276071967642	-1.032658879879
H	1.890097752879	3.763735381722	-2.262066047569
H	0.367727139671	3.418394671131	-4.216135452528
H	-1.481933761599	1.722456599230	-4.079258350417
H	-1.739150265351	0.325505624271	-2.025003909389
H	-3.200353135629	-1.417011750610	0.027395913989
H	-4.105321196707	-3.260651965704	-1.420962258190
H	-2.533845399435	-4.702186735221	-2.740195707900
H	-0.061897853997	-4.300947117152	-2.620766538864
H	1.581540823968	-3.928296290633	0.330008278557
H	4.016469442641	-3.401705021510	0.595206442777

3.

C	3.436093134290	-3.697833031584	-1.801849853898
C	2.044467901923	-3.756018968264	-1.662529899409
C	1.281709637214	-2.650556200750	-1.201329967024
C	2.028045603781	-1.485357715231	-0.900186623321
C	3.421874533920	-1.416357897798	-1.026327723575
C	4.143387402216	-2.531572098577	-1.470548838678



H	5.238028006322	-2.489608593615	-1.572290063921
H	3.934203284942	-0.471251211998	-0.789905270523
H	1.521189001506	-0.530560884871	-0.701827955558
C	-0.186978137246	-2.775440642976	-0.931122298107
C	-0.841328217670	-3.981511097279	-1.296424970894
C	-2.230303726660	-4.136227417956	-1.250467601347
C	-3.036834702757	-3.064516301134	-0.850259398981
C	-2.422842061923	-1.868829665378	-0.448772747456
C	-1.025128992078	-1.705814016662	-0.479219615402
Bi	-0.252356533896	0.103922350303	0.751605030928
Br	-2.638463970529	1.157757444770	1.385992454930
C	0.035706663699	1.426566799736	-1.111559566242
C	-0.629781867868	1.102911798250	-2.306297185632
C	-0.364711284184	1.819667897686	-3.483963367246
C	0.584613707257	2.853788916052	-3.473136449937
C	1.255152488119	3.177353681786	-2.286188906343
C	0.983286496867	2.479574326430	-1.087226712429
C	1.701500267887	2.847709968944	0.163362579814
C	3.112461686813	2.900050846061	0.198333756373
C	3.788213924100	3.214392786242	1.386566414006
C	3.065567707012	3.487995984560	2.559407066092
C	1.662507188155	3.453763536039	2.534867242388
C	0.984230165317	3.139509379446	1.347144153759
H	-0.117676624569	3.146950919607	1.324410486049
H	1.087221393497	3.682479126908	3.444848265149
H	3.596807865398	3.732373613271	3.491669855584
H	4.888643038797	3.239752043291	1.398778054425
H	3.679335863605	2.670858406834	-0.717583436273
H	1.987676170631	3.999468912445	-2.271056112005
H	0.801644674082	3.415668531568	-4.394407061978

H	-0.893981486405	1.561761449226	-4.414183412433
H	-1.352001852459	0.271517844986	-2.324155644707
H	-3.053657082258	-1.042644813635	-0.081016930609
H	-4.133287530343	-3.158404193198	-0.826844537798
H	-2.678995860074	-5.097422836904	-1.543987206629
H	-0.249859170071	-4.835496471314	-1.651449543046
H	1.550086229479	-4.702878730802	-1.914185389614
H	3.975749064158	-4.585133774515	-2.166552068482

Selected geometries from potential energy surface of aryl ring rotation of R<sub>2</sub>BiBr

R<sub>2</sub>BiBr (b)

1.

C	3.226430066521	-1.612599342530	-0.243104553330
C	1.916746323183	-2.121665682098	-0.207482291845
C	1.085275631585	-2.066371148845	-1.352291046591
C	1.615113254828	-1.521876912169	-2.541676215238
C	2.922411022615	-1.019150581446	-2.577493797736
C	3.729514481587	-1.056269348916	-1.427794140553
H	4.754061103238	-0.655749850696	-1.457664424249
H	3.308965091476	-0.576237132945	-3.507773813497
H	0.971427711353	-1.452407687048	-3.430785512574
C	-0.338865318152	-2.491027187228	-1.275382369443
C	-0.871388029505	-3.422012020028	-2.192636921255
C	-2.222031915923	-3.794001643549	-2.125503488848
C	-3.059123890235	-3.227989233559	-1.151103977009
C	-2.545340375090	-2.281657530673	-0.246969714602
C	-1.192472203617	-1.912493685024	-0.302475815542
Bi	-0.311374178748	-0.243344768223	1.028727361159
Br	-2.702729227503	0.794565354583	1.673851796363
C	0.025490059852	1.064668574578	-0.832069640051

C	-0.770138257465	0.876767227810	-1.974627756684
C	-0.447291207050	1.518817662216	-3.180286989743
C	0.689284122002	2.340898102689	-3.250134945515
C	1.476213307587	2.545509778813	-2.109627786476
C	1.146261283727	1.929288957295	-0.879945520853
C	1.964623497562	2.209638121328	0.330166745857
C	3.372160544076	2.100860043484	0.303158260855
C	4.132650094830	2.347509463992	1.454916203272
C	3.501307702646	2.713369052772	2.655266712806
C	2.104189356569	2.842710842492	2.692716568588
C	1.342225096395	2.597954005982	1.540013501685
H	0.249691307967	2.742320444726	1.562711508953
H	1.601159131663	3.148435160644	3.622675591884
H	4.099277770769	2.904472383723	3.559186123907
H	5.228299459735	2.246482499579	1.417700566430
H	3.864955246279	1.791922404037	-0.630518893516
H	2.346659058169	3.218704540007	-2.152750530628
H	0.955204901027	2.839355151710	-4.194923574397
H	-1.079719841799	1.368830049416	-4.069067577909
H	-1.642257805178	0.205641974388	-1.931981360219
H	-3.213530554498	-1.802304071695	0.487531131098
H	-4.121369563388	-3.513505187530	-1.101016597367
H	-2.622956811453	-4.529981944483	-2.839104856779
H	-0.210031518533	-3.866264164081	-2.953163841918
H	1.545038429916	-2.618101127206	0.703654164581
H	3.857199640981	-1.661351546294	0.657210716929

2.

C	2.900950017639	-1.388419632664	0.544868143276
C	1.612815970302	-1.902197668358	0.318011870251

C	1.046255345270	-1.897332210056	-0.980343841229
C	1.820901985166	-1.396195793187	-2.047961881284
C	3.107757689755	-0.890774261242	-1.820069199236
C	3.649421798280	-0.876603902852	-0.523797791640
H	4.650043348786	-0.457099890895	-0.344605888089
H	3.686407407141	-0.480006815736	-2.661378481298
H	1.382300620099	-1.360879384654	-3.056324174675
C	-0.349288182586	-2.360094534501	-1.197918895519
C	-0.645494461620	-3.310629519636	-2.199032961015
C	-1.962788044990	-3.744441929885	-2.404784848110
C	-3.003746149021	-3.225581204972	-1.619259944028
C	-2.726324245337	-2.260797197236	-0.635287807280
C	-1.409023088072	-1.826037632430	-0.424000590745
Bi	-0.922745934012	-0.116010921815	1.048334309958
Br	-3.448607802992	0.784560130383	1.097882573426
C	-0.241616025006	1.214231943514	-0.738373595700
C	-1.169328293533	1.130321954132	-1.794096856254
C	-0.872224014529	1.600974345631	-3.079547527937
C	0.392089610356	2.155329877906	-3.316588095557
C	1.309106097150	2.264849657486	-2.268261789581
C	1.040901638985	1.804220205682	-0.950786165597
C	2.053882349007	2.096765198248	0.115599932429
C	3.341284173616	2.594503389810	-0.214294194020
C	4.346168963874	2.765994362439	0.745418304678
C	4.116273582993	2.433671436291	2.089042392123
C	2.852191784253	1.947310400872	2.449317687940
C	1.854406097460	1.783373176082	1.479830594847
H	0.869576090053	1.453714901452	1.833034619067
H	2.630479642987	1.696801563156	3.497950216193
H	4.906765851756	2.560966322267	2.843677038731

H	5.326949810743	3.156243466176	0.433012678153
H	3.590749150129	2.838739698130	-1.254532905793
H	2.268535633397	2.750223528208	-2.488162660422
H	0.663881146155	2.525341730581	-4.316981778493
H	-1.618941714627	1.524456173741	-3.884416442898
H	-2.156704653156	0.676265525634	-1.613338597787
H	-3.550525434193	-1.818268679291	-0.051853013716
H	-4.039774601221	-3.561934820779	-1.779844665752
H	-2.176689077010	-4.494288194193	-3.181669272739
H	0.175745906788	-3.723784176717	-2.805498476037
H	1.056903606472	-2.371863716443	1.146110066762
H	3.322290403292	-1.393256900278	1.561050914596

3.

C	3.035713934643	-2.171469585407	0.425731721219
C	1.641694477039	-2.333674704803	0.358061425678
C	0.965592268881	-2.284421469044	-0.884641464566
C	1.725327874358	-2.074120345117	-2.056263505113
C	3.115546518522	-1.911870112933	-1.987510052873
C	3.775765317814	-1.960061221886	-0.747301246400
H	4.867847138804	-1.833413311459	-0.697222549379
H	3.689480421747	-1.735193960428	-2.909785765808
H	1.206362085392	-2.007322990074	-3.023998553641
C	-0.516417580113	-2.416504054311	-0.942761620996
C	-1.118366961538	-3.406831366192	-1.748463878694
C	-2.514650817471	-3.528539677978	-1.801668979604
C	-3.324304706258	-2.654038991735	-1.060052549982
C	-2.736013841635	-1.647484463349	-0.274025231034
C	-1.339541862384	-1.525659400757	-0.210790396039
Bi	-0.294517805516	0.243816923185	0.837504434878

Br	-2.553360781806	1.656940139428	1.146206007115
C	0.226004791854	1.127250037291	-1.216677385475
C	-0.503801110452	0.806450551776	-2.373844080998
C	-0.151198532025	1.373053276517	-3.609099151253
C	0.930387449346	2.265384370387	-3.688053337010
C	1.654609676971	2.595773924215	-2.533275267302
C	1.309969545480	2.031196493235	-1.287019404124
C	2.075696668686	2.380262502818	-0.050913480860
C	1.730569624487	3.515439004795	0.712627788720
C	2.411944372961	3.804483937051	1.905303052512
C	3.446734377635	2.965605499790	2.349212924986
C	3.799121356241	1.835706450692	1.594067566631
C	3.119420527581	1.544536955635	0.401234537477
H	3.385337796840	0.653854594664	-0.187431432021
H	4.608167464586	1.172075133161	1.936634185460
H	3.977038366119	3.191926885156	3.286711455022
H	2.127170931039	4.688842548973	2.495483300903
H	0.907340786760	4.161532819736	0.371644655306
H	2.501127133071	3.297793080544	-2.589028373563
H	1.210132992607	2.710628281988	-4.655189860504
H	-0.726412248656	1.119371739777	-4.513139991902
H	-1.354350239214	0.109491050177	-2.313599743827
H	-3.371623640314	-0.929022368839	0.269815910837
H	-4.420795341367	-2.744901381769	-1.103092202899
H	-2.972188747541	-4.311598513979	-2.425430492727
H	-0.478360510158	-4.095283189611	-2.322542646995
H	1.068292646253	-2.554767057909	1.272541766444
H	3.544722180729	-2.222878033412	1.400170912401

### Coordinates of transition state geometries of R<sub>2</sub>BiBr conformation

C	2.538206325873	-3.296217719264	-0.991856776765
C	1.148802128547	-3.373896537314	-0.951614417587
C	0.353078110523	-2.414792943694	-0.284266126813
C	1.073690820489	-1.375586494558	0.330248052109
C	2.463643367647	-1.284336076092	0.304815204605
C	3.213956016893	-2.250269059058	-0.361705768559
H	4.302514489626	-2.189372072119	-0.390711125990
H	2.949387285161	-0.446836010898	0.807681969702
H	0.575758958988	-0.561501570818	0.857824658047
C	-1.137837445441	-2.528693937138	-0.250551655780
C	-1.734142130188	-3.631532879700	-0.900788438630
C	-3.108636840005	-3.839831672022	-0.932840547654
C	-3.956865347095	-2.936583501646	-0.299670820877
C	-3.398751490948	-1.837525853167	0.352579484089
C	-2.016656671113	-1.606183264303	0.385988679404
Bi	-1.437967886272	0.274384316811	1.577454519086
Br	-3.876670182761	1.313631317729	1.877452035303
C	-0.996494466365	1.406402886138	-0.347725677574
C	-1.717491202245	1.121076006204	-1.510448290567
C	-1.393527508942	1.742012472675	-2.718271759388
C	-0.329840274214	2.645860804594	-2.770650655423
C	0.396226485209	2.934576513757	-1.616571365557
C	0.062654027910	2.332244432921	-0.391744107695
C	0.839063485824	2.655318067610	0.829612211743
C	2.237340506871	2.526856533491	0.851865988238
C	2.958874758935	2.792415688086	2.016396211797
C	2.296449925232	3.198663778671	3.177882639747
C	0.908290075236	3.348341649336	3.164939075225

C	0.185463922263	3.080466444821	2.000721420888
H	-0.896116383083	3.240486766510	1.979395459813
H	0.384434809464	3.685107925309	4.060885139444
H	2.861860303709	3.405041217191	4.087735464698
H	4.044352029548	2.678222051424	2.018930634650
H	2.752886063302	2.195850069836	-0.051809703016
H	1.218205487537	3.652815208681	-1.650176161251
H	-0.067657014455	3.131153159183	-3.712305469769
H	-1.966559654372	1.514069637111	-3.618813320033
H	-2.532153434363	0.394474009163	-1.480486083052
H	-4.070129642676	-1.127636485986	0.841586911640
H	-5.038889079401	-3.078725863669	-0.309055977635
H	-3.508820463166	-4.711401837753	-1.453566016853
H	-1.110209004838	-4.364992406452	-1.407319750280
H	0.683420184337	-4.213783446904	-1.462367772797
H	3.097472052817	-4.067224824696	-1.524534970681

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