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ELECTRONIC SUPPLEMENTARY INFORMATION

Relativistic effects on the Aromaticity of $E_3M_3H_3$ (E = C - Pb; M = N - Bi) Benzene Analogues

Ricardo Pino-Rios[a], Alejandro Vásquez-Espinal[b], Luis Alvarez-Thon[c,*] and William Tiznado[b,*]

[a]Laboratorio de Química Teórica, Facultad de Química y Biología, Universidad de Santiago de Chile (USACH), Av. Libertador Bernardo O'Higgins 3363, Santiago, Estación Central, Región Metropolitana, Chile.

[b]Departamento de Química, Facultad de Ciencias Exactas, Computational and Theoretical Chemistry Group, Universidad Andres Bello (UNAB), Av. República 275, Santiago, Región Metropolitana, Chile

[c]Facultad de Ingeniería, Universidad Central de Chile, Toesca, Santiago, 1783, Chile

Table S1. E-M bond lengths (in Å) obtained at the non-relativistic (NR), scalar (SR) and spin-orbit (SO) relativistic (ZORA)/BP86/TZ2P level.

System	E-M			E-H		
	NR	**SR**	**SO**	**NR**	**SR**	**SO**
C_6H_6	1.41	1.41	1.40	1.08	1.08	1.09
$C_3N_3H_3$	1.34	1.34	1.34	1.12	1.12	1.09
$C_3P_3H_3$	1.72	1.72	1.74	1.13	1.13	1.10
$C_3As_3H_3$	1.86	1.86	1.86	1.10	1.10	1.10
$C_3Sb_3H_3$	2.06	2.06	2.06	1.10	1.10	1.10
$C_3Bi_3H_3$	2.14	2.15	2.15	1.09	1.10	1.10
$Si_3N_3H_3$	1.70	1.70	1.66	1.51	1.50	1.48
$Si_3P_3H_3$	2.15	2.15	2.15	1.49	1.49	1.49
$Si_3As_3H_3$	2.26	2.26	2.26	1.50	1.50	1.50
$Si_3Sb_3H_3$	2.48	2.48	2.48	1.50	1.50	1.50
$Si_3Bi_3H_3$	2.55	2.56	2.57	1.50	1.51	1.51
$Ge_3N_3H_3$	1.79	1.79	1.79	1.54	1.53	1.53
$Ge_3P_3H_3$	2.23	2.22	2.22	1.55	1.55	1.55
$Ge_3As_3H_3$	2.33	2.33	2.33	1.56	1.55	1.55
$Ge_3Sb_3H_3$	2.54	2.53	2.53	1.56	1.56	1.56
$Ge_3Bi_3H_3$	2.60	2.61	2.63	1.56	1.56	1.57
$Sn_3N_3H_3$	2.01	2.01	2.01	1.74	1.72	1.72
$Sn_3P_3H_3$	2.43	2.42	2.42	1.74	1.74	1.73
$Sn_3As_3H_3$	2.53	2.52	2.52	1.75	1.74	1.74
$Sn_3Sb_3H_3$	2.72	2.71	2.72	1.75	1.74	1.74
$Sn_3Bi_3H_3$	2.78	2.79	2.83	1.75	1.75	1.76
$Pb_3N_3H_3$	2.09	2.11	2.11	1.78	1.79	1.78
$Pb_3P_3H_3$	2.50	2.50	2.50	1.78	1.81	1.80
$Pb_3As_3H_3$	2.59	2.60	2.59	1.78	1.81	1.80
$Pb_3Sb_3H_3$	2.77	2.79	2.79	1.78	1.82	1.81
$Pb_3Bi_3H_3$	2.83	2.87	2.92	1.78	1.82	1.83

Table S2. Ionization potential (IP), electron affinity (EA) and Mulliken electronegativity (χ) values (in eV) at the non-relativistic (NR), scalar (SR) and spin-orbit (SO) relativistic (ZORA)/BP86/TZ2P level.

Atom	NR			SR			SO		
	IP	**EA**	**χ**	**IP**	**EA**	**χ**	**IP**	**EA**	**χ**
C	11.0	0.9	5.9	11.0	0.9	5.9	11.0	0.9	5.9
Si	7.9	1.1	4.5	7.8	1.1	4.5	7.9	1.1	4.5
Ge	7.6	1.1	4.4	7.6	1.1	4.3	7.7	1.0	4.3
Sn	7.1	1.2	4.2	7.0	1.1	4.1	7.3	0.9	4.1
Pb	6.9	1.2	4.1	6.7	1.1	3.9	7.5	0.4	3.9
N	13.7	1.7	7.7	13.7	1.7	7.7	13.7	1.7	7.7
P	9.8	2.0	5.9	9.8	2.0	5.9	9.8	2.0	5.9
As	9.3	1.9	5.6	9.3	1.9	5.6	9.1	1.8	5.4
Sb	8.5	2.0	5.2	8.5	1.9	5.2	8.1	1.6	4.9
Bi	8.2	2.0	5.1	8.1	1.8	4.9	7.1	1.1	4.1

Table S3 NICS(1)$_{zz}$ values obtained at the non-relativistic (NR), scalar (SR) and spin-orbit (SO) relativistic (ZORA)/BP86/TZ2P level.

System	NICS(1)$_{zz}$ (ppm)		
	NR	SR	SO
C_6H_6	-28.15	-28.17	-28.55
$C_3N_3H_3$	-25.02	-25.02	-24.86
$C_3P_3H_3$	-21.89	-21.88	-21.94
$C_3As_3H_3$	-20.12	-20.26	-20.24
$C_3Sb_3H_3$	-15.08	-15.47	-15.05
$C_3Bi_3H_3$	-12.56	-13.80	-9.17
$Si_3N_3H_3$	-4.38	-4.32	-1.64
$Si_3P_3H_3$	-7.52	-7.43	-7.42
$Si_3As_3H_3$	-7.23	-7.13	-7.03
$Si_3Sb_3H_3$	-9.11	-8.92	-8.06
$Si_3Bi_3H_3$	-9.38	-8.92	-1.15
$Ge_3N_3H_3$	-0.86	-0.60	-0.58
$Ge_3P_3H_3$	-7.40	-7.22	-7.18
$Ge_3As_3H_3$	-6.80	-6.55	-6.40
$Ge_3Sb_3H_3$	-7.75	-7.30	-6.16
$Ge_3Bi_3H_3$	-8.36	-6.99	2.59
$Sn_3N_3H_3$	3.92	4.84	4.87
$Sn_3P_3H_3$	-1.54	-1.22	-1.13
$Sn_3As_3H_3$	-1.78	-1.45	-1.28
$Sn_3Sb_3H_3$	-3.16	-2.55	-1.47
$Sn_3Bi_3H_3$	-4.25	-2.51	6.26
$Pb_3N_3H_3$	6.09	10.50	10.33
$Pb_3P_3H_3$	0.60	2.60	2.81
$Pb_3As_3H_3$	0.45	2.26	2.48
$Pb_3Sb_3H_3$	-0.62	1.52	2.82
$Pb_3Bi_3H_3$	-1.34	1.69	10.25

Table S4. Diatropic (Dia) and paratropic (Para) contributions of the ring current for all pnictogen benzene analogues using BP86 with a relativistic triple-ζ quality basis set augmented with diffuse functions. Relativistic effects are treated with the four-component Dirac equation through scalar and spin-orbit effects.

System	NR		SR		SO	
	Dia	**Para**	**Dia**	**Para**	**Dia**	**Para**
C_6H_6	16.7	-4.9	16.7	-4.9	16.7	-4.9
$C_3N_3H_3$	14.8	-5.3	14.8	-5.3	14.8	-5.3
$C_3P_3H_3$	15.3	-4.5	15.2	-4.5	15.3	-4.5
$C_3As_3H_3$	65.4	-54.3	65.4	-54.3	65.7	-54.5
$C_3Sb_3H_3$	15.4	-4.5	15.5	-4.5	15.6	-4.8
$C_3Bi_3H_3$	14.8	-4.4	15.5	-4.2	14.0	-5.7
$Si_3N_3H_3$	6.2	-3.9	6.2	-3.9	6.2	-3.9
$Si_3P_3H_3$	10.7	-4.3	10.6	-4.3	10.6	-4.3
$Si_3As_3H_3$	11.7	-4.4	11.6	-4.3	11.7	-4.5
$Si_3Sb_3H_3$	13.7	-4.4	13.6	-4.2	13.8	-4.8
$Si_3Bi_3H_3$	14.2	-4.3	14.0	-4.2	11.8	-6.5
$Ge_3N_3H_3$	8.1	-5.5	8.1	-5.6	8.1	-5.6
$Ge_3P_3H_3$	12.2	-5.1	12.0	-5.0	12.1	-5.1
$Ge_3As_3H_3$	12.8	-5.0	12.6	-4.9	12.7	-5.1
$Ge_3Sb_3H_3$	14.2	-4.8	13.8	-4.7	13.8	-5.3
$Ge_3Bi_3H_3$	14.3	-4.8	13.7	-4.6	10.3	-7.0
$Sn_3N_3H_3$	8.3	-6.2	8.2	-6.5	8.2	-6.6
$Sn_3P_3H_3$	12.1	-5.9	11.8	-5.9	11.8	-5.9
$Sn_3As_3H_3$	12.7	-5.8	12.2	-5.7	12.3	-5.8
$Sn_3Sb_3H_3$	14.0	-5.6	13.3	-5.4	13.2	-5.8
$Sn_3Bi_3H_3$	15.1	-5.2	13.2	-5.3	9.3	-6.7
$Pb_3N_3H_3$	8.5	-6.8	7.4	-7.6	7.8	-7.9
$Pb_3P_3H_3$	12.7	-6.5	11.3	-6.3	11.3	-6.5
$Pb_3As_3H_3$	13.2	-6.4	11.5	-6.0	11.6	-6.2
$Pb_3Sb_3H_3$	14.5	-6.4	12.2	-5.7	11.7	-6.0
$Pb_3Bi_3H_3$	14.3	-6.0	11.6	-5.5	7.0	-6.7

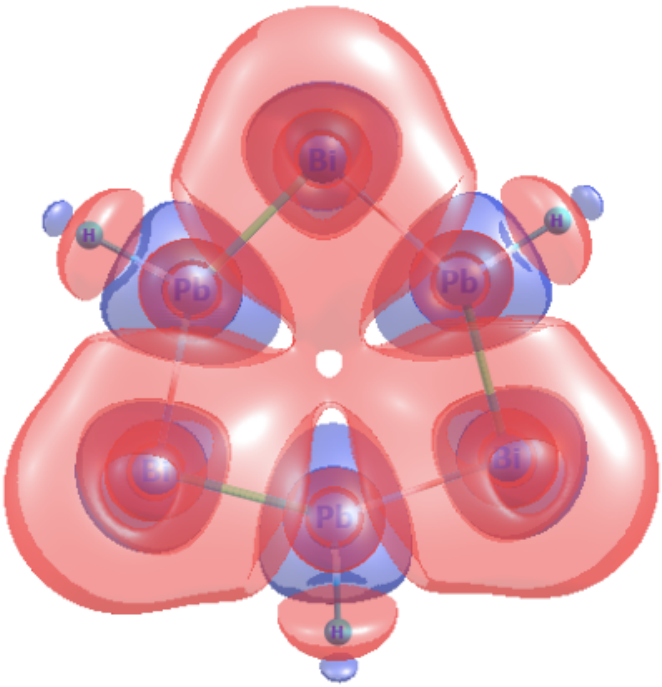

Figure S1. Plot of the electron-density difference between SO (relativistic) and NR (nonrelativistic) calculations of $Pb_3Bi_3H_3$: positive (blue) and negative (red) values, show increase and depletion in the electron density. Electron- density calculations were performed on the geometry of the neutral species. Bond lengths are almost similar in SO and NR computations.

CARTESIAN COORDINATES AT ZORA/BP86/TZ2P LEVEL INCLUDING SPIN-ORBIT RELATIVISTIC EFFECTS

C_6H_6

C	-0.698507000	1.209850000	0.000000000
C	0.698507000	1.209850000	0.000000000
C	1.397014000	0.000000000	0.000000000
C	0.698507000	-1.209850000	0.000000000
C	-0.698507000	-1.209850000	0.000000000
C	-1.397014000	0.000000000	0.000000000
H	-1.243715000	2.154177000	0.000000000
H	1.243715000	2.154177000	0.000000000
H	2.487429000	0.000000000	0.000000000
H	1.243715000	-2.154177000	0.000000000
H	-1.243715000	-2.154177000	0.000000000
H	-2.487429000	0.000000000	0.000000000

$C_3N_3H_3$

N	-0.689182000	1.193698000	0.000000000
C	0.648089000	1.122523000	0.000000000
N	1.378364000	0.000000000	0.000000000
C	0.648089000	-1.122523000	0.000000000
N	-0.689182000	-1.193698000	0.000000000
C	-1.296178000	0.000000000	0.000000000
H	1.194342000	2.068661000	0.000000000
H	1.194342000	-2.068661000	0.000000000
H	-2.388684000	0.000000000	0.000000000

$C_3P_3H_3$

P	-0.925065000	1.602259000	0.000000000
C	0.797146000	1.380697000	0.000000000
P	1.850129000	0.000000000	0.000000000
C	0.797146000	-1.380697000	0.000000000

P	-0.925065000	-1.602259000	0.000000000
C	-1.594292000	0.000000000	0.000000000
H	1.345380000	2.330267000	0.000000000
H	1.345380000	-2.330267000	0.000000000
H	-2.690760000	0.000000000	0.000000000

$C_3As_3H_3$

As	-0.994881000	1.723184000	0.000000000
C	0.847949000	1.468691000	0.000000000
As	1.989761000	0.000000000	0.000000000
C	0.847949000	-1.468691000	0.000000000
As	-0.994881000	-1.723184000	0.000000000
C	-1.695899000	0.000000000	0.000000000
H	1.396379000	2.418600000	0.000000000
H	1.396379000	-2.418600000	0.000000000
H	-2.792759000	0.000000000	0.000000000

$C_3Sb_3H_3$

Sb	-1.105459000	1.914710000	0.000000000
C	0.931114000	1.612737000	0.000000000
Sb	2.210917000	0.000000000	0.000000000
C	0.931114000	-1.612737000	0.000000000
Sb	-1.105459000	-1.914710000	0.000000000
C	-1.862228000	0.000000000	0.000000000
H	1.480147000	2.563690000	0.000000000
H	1.480147000	-2.563690000	0.000000000
H	-2.960294000	0.000000000	0.000000000

$C_3Bi_3H_3$

Bi	-1.159564000	2.008424000	0.000000000
C	0.967931000	1.676505000	0.000000000
Bi	2.319128000	0.000000000	0.000000000
C	0.967931000	-1.676505000	0.000000000

Bi	-1.159564000	-2.008424000	0.000000000
C	-1.935861000	0.000000000	0.000000000
H	1.517994000	2.629243000	0.000000000
H	1.517994000	-2.629243000	0.000000000
H	-3.035988000	0.000000000	0.000000000

$Si_3N_3H_3$

N	-0.856794000	1.484010000	0.000000000
Si	0.803866000	1.392337000	0.000000000
N	1.713587000	0.000000000	0.000000000
Si	0.803866000	-1.392337000	0.000000000
N	-0.856794000	-1.484010000	0.000000000
Si	-1.607733000	0.000000000	0.000000000
H	-3.087673000	0.000000000	0.000000000
H	1.543837000	-2.674003000	0.000000000
H	1.543837000	2.674003000	0.000000000

$Si_3P_3H_3$

P	1.167260000	2.021763000	0.000000000
Si	-0.950168000	1.645703000	0.000000000
P	-2.334564000	0.000000000	0.000000000
Si	-0.950168000	-1.645703000	0.000000000
P	1.167260000	-2.021763000	0.000000000
Si	1.900350000	0.000000000	0.000000000
H	3.393299000	0.000000000	0.000000000
H	-1.696634000	-2.938643000	0.000000000
H	-1.696634000	2.938643000	0.000000000

$Si_3As_3H_3$

As	1.232815000	2.135308000	0.000000000
Si	-0.987017000	1.709518000	0.000000000
As	-2.465694000	0.000000000	0.000000000
Si	-0.987017000	-1.709518000	0.000000000

As	1.232815000	-2.135308000	0.000000000
Si	1.974043000	0.000000000	0.000000000
H	3.472169000	0.000000000	0.000000000
H	-1.736057000	-3.006948000	0.000000000
H	-1.736057000	3.006948000	0.000000000

$Si_3Sb_3H_3$

Sb	-1.353209000	2.343826000	0.000000000
Si	1.075722000	1.863205000	0.000000000
Sb	2.706417000	0.000000000	0.000000000
Si	1.075722000	-1.863205000	0.000000000
Sb	-1.353209000	-2.343826000	0.000000000
Si	-2.151444000	0.000000000	0.000000000
H	-3.653171000	0.000000000	0.000000000
H	1.826586000	-3.163739000	0.000000000
H	1.826586000	3.163739000	0.000000000

$Si_3Bi_3H_3$

Bi	-1.411352000	2.444533000	0.000000000
Si	1.107853000	1.918857000	0.000000000
Bi	2.822703000	0.000000000	0.000000000
Si	1.107853000	-1.918857000	0.000000000
Bi	-1.411352000	-2.444533000	0.000000000
Si	-2.215706000	0.000000000	0.000000000
H	-3.724502000	0.000000000	0.000000000
H	1.862251000	-3.225513000	0.000000000
H	1.862251000	3.225513000	0.000000000

$Ge_3N_3H_3$

N	-0.932904000	1.615837000	0.000000000
Ge	0.850422000	1.472974000	0.000000000
N	1.865807000	0.000000000	0.000000000
Ge	0.850422000	-1.472974000	0.000000000

N	-0.932904000	-1.615837000	0.000000000
Ge	-1.700844000	0.000000000	0.000000000
H	-3.231766000	0.000000000	0.000000000
H	1.615883000	-2.798792000	0.000000000
H	1.615883000	2.798792000	0.000000000

$Ge_3P_3H_3$

P	-1.206349000	2.089457000	0.000000000
Ge	0.981096000	1.699308000	0.000000000
P	2.412697000	0.000000000	0.000000000
Ge	0.981096000	-1.699308000	0.000000000
P	-1.206349000	-2.089457000	0.000000000
Ge	-1.962192000	0.000000000	0.000000000
H	-3.508020000	0.000000000	0.000000000
H	1.754010000	-3.038035000	0.000000000
H	1.754010000	3.038035000	0.000000000

$Ge_3As_3H_3$

As	-1.267852000	2.195985000	0.000000000
Ge	1.016786000	1.761124000	0.000000000
As	2.535705000	0.000000000	0.000000000
Ge	1.016786000	-1.761124000	0.000000000
As	-1.267852000	-2.195985000	0.000000000
Ge	-2.033571000	0.000000000	0.000000000
H	-3.585990000	0.000000000	0.000000000
H	1.792995000	-3.105559000	0.000000000
H	1.792995000	3.105559000	0.000000000

$Ge_3Sb_3H_3$

Sb	-1.383819000	2.396845000	0.000000000
Ge	1.096204000	1.898681000	0.000000000
Sb	2.767638000	0.000000000	0.000000000
Ge	1.096204000	-1.898681000	0.000000000

Sb	-1.383819000	-2.396845000	0.000000000
Ge	-2.192408000	0.000000000	0.000000000
H	-3.749356000	0.000000000	0.000000000
H	1.874678000	-3.247038000	0.000000000
H	1.874678000	3.247038000	0.000000000

$Ge_3Bi_3H_3$

Bi	-1.448427000	2.508749000	0.000000000
Ge	1.124865000	1.948324000	0.000000000
Bi	2.896854000	0.000000000	0.000000000
Ge	1.124865000	-1.948324000	0.000000000
Bi	-1.448427000	-2.508749000	0.000000000
Ge	-2.249731000	0.000000000	0.000000000
H	-3.818139000	0.000000000	0.000000000
H	1.909069000	-3.306605000	0.000000000
H	1.909069000	3.306605000	0.000000000

$Sn_3N_3H_3$

N	-1.048684000	1.816374000	0.000000000
Sn	0.949489000	1.644563000	0.000000000
N	2.097368000	0.000000000	0.000000000
Sn	0.949489000	-1.644563000	0.000000000
N	-1.048684000	-1.816374000	0.000000000
Sn	-1.898978000	0.000000000	0.000000000
H	-3.622229000	0.000000000	0.000000000
H	1.811114000	-3.136942000	0.000000000
H	1.811114000	3.136942000	0.000000000

$Sn_3P_3H_3$

P	-1.317055000	2.281207000	0.000000000
Sn	1.064114000	1.843100000	0.000000000
P	2.634111000	0.000000000	0.000000000
Sn	1.064114000	-1.843100000	0.000000000

P	-1.317055000	-2.281207000	0.000000000
Sn	-2.128228000	0.000000000	0.000000000
H	-3.862959000	0.000000000	0.000000000
H	1.931480000	-3.345421000	0.000000000
H	1.931480000	3.345421000	0.000000000

$Sn_3As_3H_3$

As	-1.376134000	2.383534000	0.000000000
Sn	1.096082000	1.898470000	0.000000000
As	2.752268000	0.000000000	0.000000000
Sn	1.096082000	-1.898470000	0.000000000
As	-1.376134000	-2.383534000	0.000000000
Sn	-2.192164000	0.000000000	0.000000000
H	-3.933192000	0.000000000	0.000000000
H	1.966596000	-3.406244000	0.000000000
H	1.966596000	3.406244000	0.000000000

$Sn_3Sb_3H_3$

Sb	-1.489456000	2.579813000	0.000000000
Sn	1.169052000	2.024858000	0.000000000
Sb	2.978911000	0.000000000	0.000000000
Sn	1.169052000	-2.024858000	0.000000000
Sb	-1.489456000	-2.579813000	0.000000000
Sn	-2.338104000	0.000000000	0.000000000
H	-4.082147000	0.000000000	0.000000000
H	2.041073000	-3.535243000	0.000000000
H	2.041073000	3.535243000	0.000000000

$Sn_3Bi_3H_3$

Bi	-1.558208000	2.698896000	0.000000000
Sn	1.196730000	2.072796000	0.000000000
Bi	3.116417000	0.000000000	0.000000000
Sn	1.196730000	-2.072796000	0.000000000

Bi	-1.558208000	-2.698896000	0.000000000
Sn	-2.393459000	0.000000000	0.000000000
H	-4.150665000	0.000000000	0.000000000
H	2.075332000	-3.594581000	0.000000000
H	2.075332000	3.594581000	0.000000000

$Pb_3N_3H_3$

N	-1.109952000	1.922493000	0.000000000
Pb	0.989649000	1.714122000	0.000000000
N	2.219903000	0.000000000	0.000000000
Pb	0.989649000	-1.714122000	0.000000000
N	-1.109952000	-1.922493000	0.000000000
Pb	-1.979298000	0.000000000	0.000000000
H	-3.762768000	0.000000000	0.000000000
H	1.881384000	-3.258652000	0.000000000
H	1.881384000	3.258652000	0.000000000

$Pb_3P_3H_3$

P	-1.359237000	2.354268000	0.000000000
Pb	1.095459000	1.897391000	0.000000000
P	2.718474000	0.000000000	0.000000000
Pb	1.095459000	-1.897391000	0.000000000
P	-1.359237000	-2.354268000	0.000000000
Pb	-2.190918000	0.000000000	0.000000000
H	-3.986831000	0.000000000	0.000000000
H	1.993415000	-3.452697000	0.000000000
H	1.993415000	3.452697000	0.000000000

$Pb_3As_3H_3$

As	-1.415929000	2.452460000	0.000000000
Pb	1.126818000	1.951706000	0.000000000
As	2.831857000	0.000000000	0.000000000
Pb	1.126818000	-1.951706000	0.000000000

As	-1.415929000	-2.452460000	0.000000000
Pb	-2.253636000	0.000000000	0.000000000
H	-4.057446000	0.000000000	0.000000000
H	2.028723000	-3.513852000	0.000000000
H	2.028723000	3.513852000	0.000000000

$Pb_3Sb_3H_3$

Sb	-1.529542000	2.649244000	0.000000000
Pb	1.195814000	2.071210000	0.000000000
Sb	3.059083000	0.000000000	0.000000000
Pb	1.195814000	-2.071210000	0.000000000
Sb	-1.529542000	-2.649244000	0.000000000
Pb	-2.391627000	0.000000000	0.000000000
H	-4.199686000	0.000000000	0.000000000
H	2.099843000	-3.637035000	0.000000000
H	2.099843000	3.637035000	0.000000000

$Pb_3Bi_3H_3$

Bi	-1.614096000	2.795696000	0.000000000
Pb	1.227098000	2.125396000	0.000000000
Bi	3.228192000	0.000000000	0.000000000
Pb	1.227098000	-2.125396000	0.000000000
Bi	-1.614096000	-2.795696000	0.000000000
Pb	-2.454196000	0.000000000	0.000000000
H	-4.284485000	0.000000000	0.000000000
H	2.142242000	-3.710473000	0.000000000
H	2.142242000	3.710473000	0.000000000