SUPPLEMENTARY MATERIALS

to

"Electronic properties of $PbX_3CH_3NH_3$ (X=Cl, Br, I) compounds for photovoltaic and photocatalytic applications"

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1. Computed cell parameters.

	$PbCl_3$	$PbBr_3$			PbI_3		
	Cub.	Cub.	Tet.		Cub.	Tet.	
	a	***a***	***a'***	***c'***	***a***	***a'***	***c'***
PBE	5.722	6.024	8.402	12.097	6.441	8.983	12.845
PBE-D	5.652	5.931	8.265	11.844	6.308	8.721	12.555
PBEsol	5.624	5.903	8.222	11.830	6.294	8.767	12.562
PBEsol-D	5.551	5.808	8.057	11.689	6.164	8.523	12.276
B3PW91	5.736	6.034	8.423	12.116	6.441	8.987	12.853
B3PW91-D	5.736	5.896	8.188	11.860	6.260	8.722	12.557
PBE0	5.632	5.996	8.372	12.041	6.441	8.931	12.787
PBE0-D	5.640	5.914	8.232	11.795	6.289	8.673	12.499
HSE	5.702	5.994	8.393	11.988	6.408	8.898	12.923
HSED	5.607	5.860	8.174	11.738	6.235	8.807	12.769
Exp	5.675	5.901	8.322	11.833	6.328	8.856	12.660

Table S1. Computed cell parameters (using CRYSTAL14 code) using several functionals. Results highlighted in grey are obtained by including the D2 dispersion correction in the calculations. The chosen method is highlighted in dark grey.

2. Data Bandgaps.

Method	Ref	$PbCl_3$	$PbBr_3$		PbI_3	
		Cub.	Cub.	Tet.	Cub.	Tet.
Exp	Ishiharabat *et al.* [1] Papavissilion *et al.* [2,3]	2.98	2.33	2.3	1.63	1.7
LDA	Even *et al.*[4]			0.54		0.98
LDA	Brivio *et al.*[5]				1.46	
LDA-SO	Brivio *et al.*[5]				0.53	
PBE	Mosconi *et al.*[6]	2.34	1.80	1.83	1.57	1.66
PBE	Giorgi *et al.*[7]				1.64	
PBE-SO	Brivio *et al.*[5]				0.52	
PBEsol	Brivio *et al.*[5]				1.2	
HSE	This work	2.81	2.31	2.56	1.89	2.10
HSE-SO	This work	1.64	1.15	1.54	0.68	1.04
GW	Umari *et al.*[8]					2.68
GW	Brivio *et al.*[5]				2.73	
GW-SO	Umari *et al.*[8]					1.67
GW-SO	Brivio *et al.*[5]				1.67	

Table S2. Data used to draw the Figure 3.

3. Data infinit dielectric constant.

Method	Ref	$PbCl_3$	$PbBr_3$		PbI_3	
		Cub.	Cub.	Tet.	Cub.	Tet.
Exp	Hirasawa *et al.*[9]		4.8		6.5	
PBE-SO	Umari *et al.*[8]					5.6
PBEsol	Brivio *et al.*[10]				6.2	
PBEsol	Brivio *et al.*[5]				6.1	
HSE	This work	3.52	4.05	4.07	5.13	5.00
HSE-SO	This work	3.78	4.37	4.36	5.82	5.62
GW-SO	Umari *et al.*[8]					7.1
GW-SO	Brivio *et al.*[5]				4.5	

Table S3. Data used to draw the Figure 4.

4. Data dielectric constant.

Method	Ref	$PbCl_3$	$PbBr_3$		PbI_3	
		Cub.	Cub.	Tet.	Cub.	Tet.
Exp	Poglitsch *et al.*[11]	23.9	25.5		28.8	
PBEsol	Brivio *et al.*[10]				24.9	
PBEsol	Brivio *et al.*[5]				25.7	
HSE-PBE0$_{D2}$	This work	12.1	13.9	15.4	17.1	17.1
HSE-SO-PBE0$_{D2}$	This work	12.4	14.2	15.7	17.8	17.7

Table S4. Data used to draw the Figure 5.

5. Data exciton binding energies.

Method	Ref	$PbCl_3$	$PbBr_3$		PbI_3	
		Cub.	Cub.	Tet.	Cub.	Tet.
Exp	Tanaka *et al.*			76		50
Exp	Hirasawa *et al.*[9]					37
Hückel						29

HSE-ε_r	This work	9.6	6.2	8.9	3.4	6.8
HSE-ε_∞	This work	114.8	72.3	127.9	37.2	79.3
HSE-SO-ε_r	This work	15.5	10.1	7.7	5.5	3.9
HSE-SO-ε_∞	This work	166.2	107.5	100.8	50.9	39.1

Table S5. Data used to draw the Figure 7.

6. Data effective masses.

Method	**Ref**	**$PbCl_3$**		**$PbBr_3$**				**PbI_3**			
		Cub.		**Cub.**		**Tet.**		**Cub.**		**Tet.**	
		m_e^*	m_h^*	m_e^*	m_h^*	m_e^*	m_h^*	m_e^*	m_h^*	m_e^*	m_h^*
PBE	Umari *et al.*[8]									0.35	0.45
PBE-SO	Umari *et al.*[8]									0.26	0.16
HSE	This work	0.19	0.25	0.16	0.19	0.39	0.26	0.13	0.17	0.31	0.27
HSE-SO	This work	0.36	0.34	0.29	0.31	0.28	0.28	0.22	0.29	0.17	0.19
GW-SO	Umari *et al.*[8]									0.18	0.24
GW-SO	Brivio *et al.*[5]							0.15	0.12		

Table S6. Data used to draw the Figure 8.

8. Infra-red Spectroscopy.

$PbCl_3$		$PbBr_3$						PbI_3					
Cub.		Cub.		Tet.				Cub.		Tet.			
$\bar{\nu}$ / cm^{-1}	Int / a.u.	$\bar{\nu}$ / cm^{-1}	Int / a.u.	$\bar{\nu}$ / cm^{-1}	Int / a.u.	$\bar{\nu}$ / cm^{-1}	Int / a.u.	$\bar{\nu}$ / cm^{-1}	Int / a.u.	$\bar{\nu}$ / cm^{-1}	Int / a.u.	$\bar{\nu}$ / cm^{-1}	Int / a.u.
55.5	8.47	29.6	7.79	6.6	0.07	303.4	19.92	20.0	3.83	14.1	0.00	301.9	0.15
61.7	23.86	36.2	2.95	12.1	0.01	307.5	0.97	29.3	5.40	16.9	0.00	308.3	6.34
64.2	3.73	41.2	12.80	27.2	0.03	912.5	459.20	32.4	3.79	22.1	0.06	912.1	345.62
64.2	20.95	41.9	3.60	28.6	0.79	913.7	0.14	34.4	10.50	24.1	0.02	915.9	10.89
78.4	38.97	47.9	5.00	31.7	0.50	920.5	13.25	38.8	19.25	27.0	0.02	916.2	2.35
95.0	14.33	53.7	18.61	35.3	0.02	922.1	0.51	40.4	34.52	27.9	0.17	917.2	3.64
97.0	11.65	84.8	52.38	39.1	28.15	933.5	97.15	54.8	13.75	28.6	6.11	928.6	52.79
109.7	18.48	87.2	207.00	39.3	32.14	935.0	224.41	65.4	38.70	28.8	108.11	929.6	34.05
112.3	201.14	90.2	25.50	40.2	0.03	935.5	86.32	73.3	110.77	29.8	160.93	930.4	59.31
120.7	250.00	100.5	201.77	44.4	28.14	936.5	18.71	75.4	164.47	33.2	77.01	931.9	5.54
145.1	244.14	106.1	195.46	44.8	13.70	1024.1	5.79	83.7	191.04	36.7	40.96	1017.8	0.02
164.1	385.92	114.8	40.03	45.5	42.96	1024.4	26.50	95.9	138.23	37.1	0.79	1017.9	34.83
173.6	60.54	124.6	49.25	48.5	45.32	1025.2	30.27	100.0	3.82	38.3	1.16	1018.5	0.00
185.4	105.73	138.4	77.64	49.3	0.20	1025.6	4.20	113.4	49.25	39.5	19.06	1018.7	25.00
187.4	84.72	143.5	91.23	52.4	6.85	1281.6	150.24	118.4	92.12	40.1	8.52	1275.1	0.06
341.4	0.65	330.3	1.24	52.9	1.87	1282.7	0.55	303.2	9.65	41.8	0.08	1276.8	0.10
934.0	39.85	922.9	49.98	53.6	4.05	1283.8	0.45	920.1	112.21	43.1	0.24	1277.6	0.04
962.1	35.33	947.9	36.73	57.6	18.30	1284.2	0.05	930.8	31.26	44.3	0.38	1279.1	34.91
1043.6	15.31	1026.9	14.39	57.8	54.30	1289.4	0.30	1013.0	11.43	45.2	4.39	1288.4	9.19
1290.5	15.45	1283.9	14.87	58.2	11.57	1290.0	0.61	1282.8	22.19	46.3	0.16	1289.1	20.95
1300.0	7.72	1293.5	7.57	58.5	3.53	1290.7	22.10	1286.9	10.45	48.0	0.01	1289.9	29.16
1449.1	29.75	1450.6	23.14	60.9	1.55	1291.1	20.75	1453.0	18.97	49.0	1.05	1291.0	8.79
1499.2	35.70	1495.9	32.71	63.3	7.15	1447.4	0.07	1493.5	40.52	49.8	266.10	1448.2	0.71
1511.2	8.99	1503.7	14.46	65.0	0.12	1448.1	40.68	1496.5	35.49	50.1	1.47	1448.3	94.29
1569.5	182.89	1552.1	173.50	65.3	451.14	1448.3	48.50	1540.2	211.28	50.3	3.36	1448.6	18.18
1646.2	117.89	1637.3	141.15	68.1	34.54	1448.8	0.10	1634.2	148.08	51.8	10.02	1449.0	95.04
1647.1	213.22	1652.8	191.86	69.6	0.23	1485.1	1.33	1645.2	200.54	53.3	0.48	1494.2	9.72
3098.7	4.49	3093.9	2.46	72.0	2.39	1486.1	0.13	3083.5	1.50	57.0	1.44	1495.1	19.86
3214.4	4.49	3207.8	3.66	74.1	6.09	1487.9	162.68	3199.0	2.87	58.7	32.95	1495.6	14.58
3222.1	2.12	3217.8	1.94	76.1	2.17	1488.8	0.05	3208.2	0.60	61.3	640.84	1495.9	31.30
3297.6	562.35	3293.6	545.62	79.1	121.69	1494.4	112.36	3319.3	506.53	63.7	14.61	1498.5	101.65
3332.3	1210.39	3340.4	1113.54	84.1	189.68	1494.5	27.89	3388.7	808.83	65.3	319.18	1498.7	13.46
3448.7	385.35	3464.7	301.75	87.5	4.80	1499.0	0.50	3438.8	504.26	65.5	61.30	1499.6	1.81
				88.4	731.38	1499.7	137.47			67.4	519.05	1500.6	5.20
				90.0	157.25	1526.6	0.91			68.5	49.52	1525.6	11.47
				92.8	4.88	1529.8	146.50			69.0	57.09	1527.3	314.83
				93.2	1.63	1533.3	312.43			74.2	4.19	1533.7	229.16
				95.0	31.77	1535.5	3.15			76.3	2.43	1534.6	127.16
				95.5	496.61	1621.0	106.84			78.6	52.05	1623.3	52.67
				98.1	26.28	1623.0	1.08			79.1	53.54	1625.9	566.05
				98.8	48.66	1628.7	0.62			80.1	2.13	1627.5	432.63

		99.8	36.19	1630.7	80.86		81.1	0.01	1630.1	468.63
		102.2	31.64	1637.4	503.21		81.6	15.99	1635.4	324.11
		102.4	52.11	1641.6	1.90		88.2	16.16	1638.4	12.61
		103.6	69.91	1648.6	0.04		88.8	5.31	1641.4	9.10
		108.3	55.93	1653.2	10.53		91.5	4.13	1644.9	96.40
		110.1	3.87	3100.1	2.53		91.8	7.29	3086.9	0.94
		118.7	44.93	3100.9	3.51		102.0	0.59	3087.1	1.24
		119.4	25.16	3101.3	1.16		102.3	0.08	3090.6	1.42
		120.8	1.04	3101.5	4.11		102.6	1.49	3091.7	1.27
		121.3	0.58	3214.8	0.00		110.8	0.02	3203.0	2.08
		134.0	40.29	3215.0	3.71		116.6	0.03	3203.4	1.79
		134.8	0.05	3215.2	12.60		118.8	23.91	3203.5	1.55
		138.8	1.17	3216.2	7.21		120.5	1.17	3203.9	1.62
		145.7	1.00	3221.1	2.86		121.3	5.66	3208.6	2.68
		146.3	0.08	3221.6	4.90		121.6	87.94	3209.0	2.37
		149.0	0.54	3224.3	1.80		121.8	67.77	3218.1	1.61
		151.0	131.31	3224.6	5.18		131.8	5.26	3220.2	1.79
		155.9	0.65	3275.2	2158.08		133.3	2.45	3304.5	437.09
		157.5	68.43	3276.5	1249.05		134.1	112.95	3305.5	279.86
		158.2	4.98	3278.4	184.70		139.0	0.25	3310.4	517.51
		159.7	115.29	3283.6	28.94		159.1	29.25	3311.1	1231.46
		161.1	0.19	3391.9	646.10		160.1	52.06	3365.5	1012.61
		165.6	0.04	3394.0	416.77		161.6	53.66	3371.0	792.44
		167.3	5.45	3398.6	1325.41		164.8	2.34	3383.6	1660.40
		186.2	575.40	3401.1	844.43		173.2	209.63	3385.7	319.53
		188.6	36.21	3430.4	974.53		175.2	53.47	3428.8	166.29
		190.7	1.07	3433.4	335.26		177.7	69.66	3430.1	180.67
		203.6	0.01	3438.8	292.31		178.2	10.56	3433.8	1595.65
		296.8	10.25	3441.3	389.62		299.6	19.78	3437.6	16.97
		300.7	3.63				301.2	6.30		

Table S7. Computed IR frequencies and intensities (on the PBE0-D geometries). Values with $I^2/\tilde{\nu}^2 > 1$ are highlighted and correspond to the transitions strongly contributing to the vibrational term in the dielectric constant.

9. Summary of values of the band gaps, exciton binding energies and dielectric constants

	E_g (no SO)	E_g (SO)	$E_b(\infty)$	$E_b(r)$	ε_∞	ε_{vib}	ε_r
$PbCl_3$-c (R)	2.81	1.64	99.3	9.2	3.79	8.6	12.1
$PbBr_3$-c (R)	2.31	1.15	62.5	5.9	4.37	9.9	13.9
PbI_3-c (R)	1.88	0.68	28.6	3.1	5.85	12.0	17.1
$PbBr_3$-t (G)	2.56	1.54	111.6	8.6	4.36	11.4	15.8
PbI_3-t (G)	2.10	1.04	62.6	6.3	5.62	12.1	17.7

10. Summary of effective masses

a. With Spin-Orbit-coupling:

Tetragonal phases

Direction	I		Br	
	h^+	e^-	h^+	e^-
100	0.20	0.18	0.28	0.27
001	0.18	0.13	0.35	0.37
110	0.20	0.18	0.27	0.27
011	0.20	0.24	0.25	0.24
111	0.19	0.16	0.29	0.29
$\bar{m}^*$	0.19	0.17	0.28	0.28

Cubic phases

Direction	I		Br		Cl	
	h^+	e^-	h^+	e^-	h^+	e^-
100	0.29	0.23	0.34	0.29	0.37	0.36
110	0.30	0.22	0.31	0.28	0.34	0.35
111	0.29	0.24	0.30	0.30	0.33	0.37
$\bar{m}^*$	0.29	0.23	0.31	0.29	0.35	0.36

b. Without Spin-Orbit-coupling:

Tetragonal phases

Direction	I		Br	
	h^+	e^-	h^+	e^-
100	0.24	1.12	0.28	0.90
001	0.42	0.16	0.37	0.28
110	0.29	1.15	0.34	1.16
011	0.22	0.21	0.24	0.25
111	0.26	0.32	0.18	0.29
$\bar{m}^*$	0.27	0.31	0.26	0.39

Cubic phases

Direction	I		Br		Cl	
	h^+	e^-	h^+	e^-	h^+	e^-
100	0.18	0.09	0.20	0.12	0.24	0.14
110	0.17	0.14	0.19	0.18	0.23	0.24
111	0.16	0.20	0.18	0.22	0.21	0.27
$\bar{m}^*$	0.17	0.13	0.19	0.16	0.23	0.20

11. Geometry Optimizations

The geometries of all structures ((c)ubic and (t)etragonal) are provided in this section. Lattice parameters are in Å, atomic positions are expressed relative to the lattice dimensions.

```
PbI3-c, constrained optimization
a=b=c 6.2887177267999999
Pb 0.0 0.0 0.0
I 0.5 0.0 0.0
I 0.0 0.5 0.0
I 0.0 0.0 0.5
N 0.4874524620054004 0.4940061548475967 0.6764940157680002
C 0.5314187159587007 0.5014580668713009 0.4442999829246972
H 0.3279499668270986 0.5116171663013986 0.7094820121784977
H 0.5667520886567985 0.6122178141067991 0.7570639838185969
H 0.5354349635685978 0.3515216315240011 0.7417592796736017
H 0.4659672075208974 0.6487549367892029 0.3800563606133025
H 0.4558479018761972 0.3637103772651002 0.3706797956764021
H 0.7031241123592977 0.4954237172940026 0.4205809092176978

PbI3-t, constrained optimization
a 8.7594521844 (a=b=8.759452)
b 8.7594524422
c 12.5965028
Pb 0.0 0.0 0.0
Pb 0.5 0.5 0.0
Pb 0.0 0.0 0.5
Pb 0.5 0.5 0.5 I 0.0 0.0 0.25
I 0.0 0.0 -0.25 I 0.5 0.5 0.25
I 0.5 0.5 -0.25
I 0.2106317239 -0.2893682761 1.74277805722871E-019
I -0.1806523254 0.3193476746 3.42728007729733E-020
I 0.3007524708 0.2007524708 1.41763902841986E-019
I -0.2989083449 -0.1989083449 2.27344383197057E-019
I -0.2860490432 0.2139509568 0.500000003
I 0.3209227279 -0.1790772721 0.500000003
I -0.1981316415 -0.2981316415 0.500000003
I 0.2022018077 0.3022018077 0.500000003
N 0.0838675659 0.4392904691 0.2161279149
N 0.4214542346 -0.0574143145 0.2125618639
N -0.0799582269 0.4418273764 -0.287463372
N -0.4147599262 -0.0544454598 -0.2863950697
C -0.0351525679 -0.4600814489 0.2623852347
C 0.4909029123 0.0639862746 0.2791115531
C -0.0099200926 -0.4375587423 -0.220568704
C 0.4889266377 0.0449431133 -0.2183032539
H 0.137152561 0.4924470706 0.153349416
H 0.1648467338 0.4122628717 0.272108407
H 0.0366037176 0.3400572362 0.1875755833
H -0.0890530338 0.4800302166 0.3282692687
H 0.0189852492 -0.3560284993 0.2914322034
H -0.1188345442 -0.4330304723 0.201074166
H 0.3786533726 -0.0108643044 0.1433880131
H 0.5000694733 -0.1393679529 0.1925474421
H 0.3322376138 -0.1086786043 0.2515516677
H -0.4635597968 0.0121069544 0.3509499342
H -0.4187670037 0.1199414424 0.2340068713
H 0.4024363748 0.146494248 0.2997406108
H -0.1221674008 0.4887615664 -0.3566683687
H -0.0017635369 0.3594371119 -0.3073757435
H -0.1697677456 0.3911410223 -0.2487182353
H 0.0349693249 -0.4901175095 -0.1487844566
H 0.0810615478 -0.3820704393 -0.2653100335
H -0.0978589398 -0.3545449563 -0.1998376659
H -0.3462044867 0.0109990764 -0.3348311938
H -0.3464835004 -0.1224877781 -0.2399774863
H -0.4817542556 -0.1220508566 -0.334573183
H 0.417518879 -0.0274873888 -0.1685592371
H -0.4364610871 0.1145108471 -0.1686377704
H 0.4187055714 0.1176164551 -0.2689083776

PbBr3-c, constrained optimization
a=b=c 0.591418218236E+01
```

```
Pb 0.0 0.0 0.0
Br -0.5 0.0 0.0
Br 0.0 -0.5 0.0
Br 0.0 0.0 -0.5
N 0.4763233 0.4914506 -0.3139409
C -0.4642825 0.4961150 0.4421872
H 0.3055355 -0.4866294 -0.2883953
H -0.4429436 -0.3827910 -0.2256062
H -0.4821039 0.3385629 -0.2415799
H 0.4718387 -0.3469639 0.3692842
H 0.4571486 0.3499914 0.3617244
H -0.2809593 0.4863351 0.4258766

PbBr3-t, constrained optimization
a=b=8.2320778
c=11.79492047
Pb  0.0    0.0    0.0
Pb -0.5   -0.5    0.0
Pb  0.0    0.0   -0.5
Pb -0.5   -0.5   -0.5
Br  0.0    0.0    0.25
Br  0.0    0.0   -0.25
Br -0.5   -0.5    0.25
Br -0.5   -0.5   -0.25
Br 0.22301217    -0.27698783    0.00000000
Br -0.18263739    0.31736261    0.00000000
Br 0.29599031    0.19599031    0.00000000
Br -0.30396357    -0.20396357    0.00000000
Br -0.27489204    0.22510796    -0.50000000
Br 0.32380009    -0.17619991    -0.50000000
Br -0.20228227    -0.30228227    -0.50000000
Br 0.19815152    0.29815152    -0.50000000
N  0.07886333    0.44980884    0.20121931
N  0.41095633    -0.05879313    0.21922723
N  -0.08612997    0.44370013    -0.28821583
N  -0.42625293    -0.07257512    -0.27060394
C  -0.02402052    -0.46008718    0.28302198
C  -0.48522838    0.05571415    0.28385675
C  0.01024893    -0.44693549    -0.21445950
C  0.46510431    0.07000121    -0.25676016
H  0.14177102    -0.47126020    0.14957322
H  0.16128913    0.37801719    0.24264084
H  0.00858528    0.37854587    0.14865149
H  -0.09042993    0.45260141    0.33479058
H  0.05470582    -0.38664816    0.33682073
H  -0.10813533    -0.38243586    0.23644737
H  0.34150122    0.00243723    0.16058250
H  0.47883826    -0.14252161    0.17563401
H  0.33460043    -0.11952833    0.27341765
H  -0.40882136    -0.01423625    0.34121167
H  -0.41167924    0.12614202    0.22478542
H  0.43590610    0.13567679    0.33297684
H  -0.14929208    -0.49031873    -0.34813503
H  -0.01335703    0.36416897    -0.33200734
H  -0.16817242    0.37846860    -0.24136435
H  0.08111099    0.47912028    -0.15606226
H  0.08942085    -0.37250606    -0.26728982
H  -0.07343486    -0.37020180    -0.16668945
H  -0.31059036    -0.03782955    -0.29284096
H  -0.41596313    -0.13706931    -0.19612296
H  -0.47023883    -0.14851485    -0.33258119
H  0.34607572    0.02782086    -0.22908267
H  -0.48268988    0.15050968    -0.19327045
H  0.45497267    0.13194159    -0.33810367

PbCl3-c, constrained optimization
a=b=c 0.563979292000E+01
```

```
Pb 0.0 0.0 0.0
Cl -0.5 0.0 0.0
Cl 0.0 -0.5 0.0
Cl 0.0 0.0 -0.5
N 0.468761 0.498906 -0.305443
C -0.463504 0.498743 0.440873
H 0.287677 -0.497966 -0.279820
H -0.465780 -0.354885 -0.218087
H -0.471200 0.349548 -0.219232
H 0.467508 -0.340124 0.359373
H 0.459870 0.341971 0.357852
H -0.270838 0.494052 0.428463
```

```
PbI3-c, unconstrained optimization
a 6.32217490 alpha 88.584465
b 6.19709604 beta 92.815823
c 6.37790877 gamma 88.217428
Pb 1.271555482731E-02 -3.535442795481E-03 3.965632303378E-02
I -4.845153412397E-01 6.095592821410E-03 -2.719740685473E-03
I -2.424422510490E-02 4.963281563581E-01 -3.535859574524E-02
I 7.082661554633E-02 -7.722102381113E-03 -4.877475900023E-01
N 4.509582620841E-01 -4.882202011204E-01 -3.387598401004E-01
C -4.500040587209E-01 4.847057183614E-01 4.566452867998E-01
H 2.972149422163E-01 -4.293695887284E-01 -3.577226541282E-01
H -4.681687915615E-01 -3.814714749393E-01 -2.461309543111E-01
H 4.497196213025E-01 3.673388168442E-01 -2.550075486376E-01
H -4.548618200951E-01 -3.590899062387E-01 3.734051755640E-01
H 4.608011791770E-01 3.671671931732E-01 3.668949251949E-01
H -2.864945252739E-01 4.264830980288E-01 4.872615472722E-01

PbI3-t, unconstrained optimization
a 8.43865375 alpha 85.448026
b 7.79704572 beta 89.960109
c 11.90148590 gamma 90.004073
Pb -1.608681759094E-02 -3.519984351563E-03 1.315280784427E-02
Pb -4.839518620181E-01 4.965043930970E-01 1.366470818820E-02
Pb 1.542079041023E-02 -3.359438586540E-03 -4.868533136542E-01
Pb 4.833428362911E-01 4.966330122075E-01 -4.864521404358E-01
Br 1.500340335724E-02 2.228080564862E-02 2.645778116141E-01
Br -1.591836986833E-02 2.223876901193E-02 -2.353662345480E-01
Br 4.837536437023E-01 -4.774962763440E-01 2.652750363364E-01
Br -4.847327803644E-01 -4.773584314365E-01 -2.347333931246E-01
Br 2.278355714139E-01 -2.772663111436E-01 1.658175418330E-02
Br -1.564100439261E-01 3.503947363083E-01 2.895734259311E-03
Br 2.722884284974E-01 2.230295853541E-01 1.680516677283E-02
Br -3.433806661813E-01 -1.494478010295E-01 3.461656115596E-03
Br -2.730256199080E-01 2.229601699459E-01 -4.831905869961E-01
Br 3.428167217609E-01 -1.492609779606E-01 -4.965835030865E-01
Br -2.285454699040E-01 -2.770475872109E-01 -4.833630851318E-01
Br 1.560042868903E-01 3.502366147798E-01 -4.970757685152E-01
N 7.615048957181E-02 4.531140695892E-01 2.246664172511E-01
C -6.733338599407E-02 -4.624569906122E-01 2.662305430423E-01
H 1.267481382080E-01 -4.750795241978E-01 1.572259348537E-01
H 1.592371820190E-01 4.358137579202E-01 2.875384719283E-01
H 5.002142268762E-02 3.334335308829E-01 1.992792946331E-01
H -1.190511631569E-01 4.546068992791E-01 3.347435600646E-01
H -3.349198755013E-02 -3.395119742431E-01 2.967130365492E-01
H -1.509873126103E-01 -4.424963452318E-01 1.967119736514E-01
N 4.227536453832E-01 -4.644119255469E-02 2.250101787470E-01
C -4.337150617607E-01 3.811981347413E-02 2.662988766154E-01
H 3.708761019896E-01 2.637985080061E-02 1.585912389312E-01
H 4.492410692270E-01 -1.650611462456E-01 1.981285181203E-01
H 3.407507352325E-01 -6.587853410380E-02 2.885310190261E-01
H -3.805801792330E-01 -4.587610146654E-02 3.336128242256E-01
H -3.511209348410E-01 6.041979151559E-02 1.962396631603E-01
H -4.679205744626E-01 1.598326312310E-01 2.983755149825E-01
N -7.700694086996E-02 4.536271723451E-01 -2.753337131640E-01
C 6.669727762172E-02 -4.620459118487E-01 -2.341085794572E-01
H -1.287300644105E-01 -4.735678590354E-01 -3.418510943458E-01
H -5.071546059178E-02 3.348511805307E-01 -3.020995216470E-01
H -1.591259369720E-01 4.345277255189E-01 -2.118399533502E-01
H 1.197639951155E-01 4.539097282733E-01 -1.667705217502E-01
H 1.492749844964E-01 -4.399637821871E-01 -3.041966689449E-01
H 3.272574354024E-02 -3.401855763664E-01 -2.021175112454E-01
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N -4.237900326404E-01 -4.681418235906E-02 -2.749725607435E-01
C 4.329724041640E-01 3.800205041394E-02 -2.333232759102E-01
H -3.737296749428E-01 2.428198091427E-02 -3.429442780106E-01
H -3.401734672637E-01 -6.322774247858E-02 -2.123872082209E-01
H -4.500455110699E-01 -1.669969060082E-01 -2.995195629410E-01
H 3.819316703952E-01 -4.414290171247E-02 -1.641420693686E-01
H 4.669839008508E-01 1.614857246573E-01 -2.037353930122E-01
H 3.486857014766E-01 5.685150024198E-02 -3.025325006047E-01

PbBr3-c, unconstrained optimization
a 5.96447237 alpha 90.349905
b 5.77117435 beta 91.294961
c 5.88224848 gamma 90.685044
Pb 1.355417081773E-02 -4.861815629931E-04 3.381241657654E-02
Br -4.838365698323E-01 -5.760749740540E-03 -3.556776655431E-03
Br -4.701234851793E-02 4.987491380980E-01 -3.220025212523E-02
Br 8.521296561525E-02 1.070253791327E-03 -4.734326234436E-01
N 4.399465065975E-01 4.932336118343E-01 -3.285187077022E-01
C -4.450199164325E-01 4.981373208612E-01 4.508223284133E-01
H 2.690449497423E-01 4.780796803237E-01 -3.488321496160E-01
H 4.724818746012E-01 -3.574182884087E-01 -2.356586558306E-01
H 4.908781695535E-01 3.545077526199E-01 -2.315319588759E-01
H 4.965835657923E-01 -3.521095922517E-01 3.550990447737E-01
H -4.846664704826E-01 3.376392440809E-01 3.588130337172E-01
H -2.649216520890E-01 -4.872127939405E-01 4.847727396032E-01

PbBr3-t, unconstrained optimization
a 8.43865375 alpha 85.448026
b 7.79704572 beta 89.960109
c 11.90148590 gamma 90.004073
Pb -1.608681759094E-02 -3.519984351563E-03 1.315280784427E-02
Pb -4.839518620181E-01 4.965043930970E-01 1.366470818820E-02
Pb 1.542079041023E-02 -3.359438586540E-03 -4.868533136542E-01
Pb 4.833428362911E-01 4.966330122075E-01 -4.864521404358E-01
Br 1.500340335724E-02 2.228080564862E-02 2.645778116141E-01
Br -1.591836986833E-02 2.223876901193E-02 -2.353662345480E-01
Br 4.837536437023E-01 -4.774962763440E-01 2.652750363364E-01
Br -4.847327803644E-01 -4.773584314365E-01 -2.347333931246E-01
Br 2.278355714139E-01 -2.772663111436E-01 1.658175418330E-02
Br -1.564100439261E-01 3.503947363083E-01 2.895734259311E-03
Br 2.722884284974E-01 2.230295853541E-01 1.680516677283E-02
Br -3.433806661813E-01 -1.494478010295E-01 3.461656115596E-03
Br -2.730256199080E-01 2.229601699459E-01 -4.831905869961E-01
Br 3.428167217609E-01 -1.492609779606E-01 -4.965835030865E-01
Br -2.285454699040E-01 -2.770475872109E-01 -4.833630851318E-01
Br 1.560042868903E-01 3.502366147798E-01 -4.970757685152E-01
N 7.615048957181E-02 4.531140695892E-01 2.246664172511E-01
C -6.733338599407E-02 -4.624569906122E-01 2.662305430423E-01
H 1.267481382080E-01 -4.750795241978E-01 1.572259348537E-01
H 1.592371820190E-01 4.358137579202E-01 2.875384719283E-01
H 5.002142268762E-02 3.334335308829E-01 1.992792946331E-01
H -1.190511631569E-01 4.546068992791E-01 3.347435600646E-01
H -3.349198755013E-02 -3.395119742431E-01 2.967130365492E-01
H -1.509873126103E-01 -4.424963452318E-01 1.967119736514E-01
N 4.227536453832E-01 -4.644119255469E-02 2.250101787470E-01
C -4.337150617607E-01 3.811981347413E-02 2.662988766154E-01
H 3.708761019896E-01 2.637985080061E-02 1.585912389312E-01
H 4.492410692270E-01 -1.650611462456E-01 1.981285181203E-01
H 3.407507352325E-01 -6.587853410380E-02 2.885310190261E-01
H -3.805801792330E-01 -4.587610146654E-02 3.336128242256E-01
H -3.511209348410E-01 6.041979151559E-02 1.962396631603E-01
H -4.679205744626E-01 1.598326312310E-01 2.983755149825E-01
N -7.700694086996E-02 4.536271723451E-01 -2.753337131640E-01
C 6.669727762172E-02 -4.620459118487E-01 -2.341085794572E-01
H -1.287300644105E-01 -4.735678590354E-01 -3.418510943458E-01
H -5.071546059178E-02 3.348511805307E-01 -3.020995216470E-01
H -1.591259369720E-01 4.345277255189E-01 -2.118399533502E-01
H 1.197639951155E-01 4.539097282733E-01 -1.667705217502E-01
H 1.492749844964E-01 -4.399637821871E-01 -3.041966689449E-01
H 3.272574354024E-02 -3.401855763664E-01 -2.021175112454E-01
N -4.237900326404E-01 -4.681418235906E-02 -2.749725607435E-01
C 4.329724041640E-01 3.800205041394E-02 -2.333232759102E-01
H -3.737296749428E-01 2.428198091427E-02 -3.429442780106E-01
H -3.401734672637E-01 -6.322774247858E-02 -2.123872082209E-01
H -4.500455110699E-01 -1.669969060082E-01 -2.995195629410E-01
H 3.819316703952E-01 -4.414290171247E-02 -1.641420693686E-01
H 4.669839008508E-01 1.614857246573E-01 -2.037353930122E-01

```
H 3.486857014766E-01 5.685150024198E-02 -3.025325006047E-01

PbCl3-c, unconstrained optimization
a 5.70612583 alpha 90.017465
b 5.47759452 beta 88.900074
c 5.62095787 gamma 90.036249
Pb 7.657462002782E-03 -6.743817175098E-04 4.718132080186E-02
Cl -4.886917770026E-01 -9.174980993197E-04 -1.057690293611E-02
Cl -6.116281690667E-02 4.992745583037E-01 -4.261306984132E-02
Cl 8.892642022943E-02 -8.136592053768E-04 -4.577551769271E-01
N 4.378247402566E-01 4.990376262231E-01 -3.177364675208E-01
C -4.452628390779E-01 4.993087587124E-01 4.453506041093E-01
H 2.583348050656E-01 4.987879891758E-01 -3.275734428964E-01
H 4.837627639927E-01 -3.483910389967E-01 -2.215802343100E-01
H 4.839785767175E-01 3.465256888672E-01 -2.217953207187E-01
H -4.983598081508E-01 -3.368980164560E-01 3.503820188030E-01
H -4.981153540962E-01 3.354445073763E-01 3.501348111177E-01
H -2.563981730302E-01 4.995604658161E-01 4.705608603184E-01
```

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