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Matrix Infrared Spectroscopic and Theoretical Studies for the Products of Lead Atom Reactions of with Ethane and Halomethanes

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Table S1: Observed and Calculated Fundamental Frequencies of CH_3CH_2-PbH Isotopomers in the Ground ^{1}A Electronic State[a]

Approximate Description	CH_3CH_2-PbH					CD_3CD_2-PbD				
	Obs[b]	B3LYP[c]		BPW91[d]		Obs[b]	B3LYP[c]		BPW91[d]	
		Freq.	Int.	Freq.	Int.		Freq.	Int.	Freq.	Int.
CH_3 aymm. str.		3086.2	40	3038.2	37		2283.8	20	2248.2	18
CH_3 aymm. str.		3053.8	12	3005.4	11		2258.2	8	2221.8	6
CH_2 asymm. str.		3047.8	39	3000.1	33		2253.6	16	2217.2	14
CH_3 sym. str.		2999.8	52	2946.2	37		2180.0	20	2141.7	16
CH_2 sym str.		2992.7	62	2938.0	77		2155.4	37	2115.2	39
Pb-H str.	1513.4, 1508.5, 1506.3	1547.7	535	1510.9	474	1086.0, 1081.5	1097.4	255	1071.2	231
CH_3 as. bend		1505.0	12	1460.2	10		1136.7	4	1105.3	4
CH_3 as. bend		1495.6	7	1451.0	6		1083.3	10	1050.3	5
CH_2 scis.		1454.3	0	1406.3	1		1081.5	9	1047.7	9
CH_3 deform		1415.3	12	1367.5	12		1067.3	8	1032.2	6
CH_2 twist		1255.2	0	1214.1	1		979.9	1	949.0	1
CH_2 wag		1190.2	19	1143.8	22		967.0	5	930.5	6
C-C str.		1015.1	11	997.0	6		886.4	6	868.5	6
CH_3 rock		964.9	6	939.2	8		715.4	7	693.4	6
CH_3 rock		918.0	4	889.9	4		662.1	2	642.1	2
CPbH bend		637.0	20	613.7	16		481.6	7	464.6	6

C-Pb str.	510.8	17	492.2	14	371.7	3	357.9	2
CH_2 rock	382.5	32	373.5	29	339.8	34	331.9	31
CH_3 tort	224.6	1	219.4	0	181.6	0	176.3	0
CCW bend	180.6	2	176.3	1	142.5	0	139.6	0
HPb tort	51.0	8	60.4	7	37.9	4	44.3	4

[a]Frequencies and infrared intensities computed with 6-311++G(3df, 3pd) are for harmonic calculations. The SDD core potential and basis set are used for Pb. [b]Observed in an argon matrix. [c]Calculated with B3LYP. [d]Calculated with BPW91. Frequencies and intensities are in cm^{-1} and km/mol. CH_3CH_2-PbH has a C_1 structure.

Table S2: Observed and Calculated Fundamental Frequencies of CH_3-PbF Isotopomers in the ^{1}A' State[a]

Approximate Description	CH_3-PbF					CD_3-PbF					$^{13}CH_3$-PbF				
	Obs[b]	B3LYP[c]		BPW91[d]		Obs[b]	B3LYP[c]		BPW91[d]		Obs[b]	B3LYP[c]		BPW91[d]	
		Freq	Int	Freq	Int		Freq	Int	Freq	Int		Freq	Int	Freq	Int
A' CH_3 as str.		3130.5	9	3085.6	8		2318.3	4	2284.9	3		3119.3	9	3074.5	8
A" CH_3 as str.		3086.9	22	3043.8	19		2282.5	11	2250.5	9		3076.0	22	3033.2	19
A' CH_3 s. str.		3016.6	21	2966.2	16		2160.0	7	2123.6	5		3013.7	21	2963.4	16
A" CH_3 bend		1449.0	7	1402.2	7		1052.3	4	1018.3	4		1445.6	7	1399.0	7
A' CH_3 bend		1444.8	5	1399.1	5		1046.3	3	1013.0	4		1441.9	5	1396.3	5
A' CH_3 deform		1173.0	0	1126.4	0		900.2	5	863.8	4		1165.5	0	1119.3	0
A' CH_3 rock		670.0	8	651.3	8		510.2	11	495.6	10		665.7	8	647.1	7
A" CH_3 rock		583.5	0	566.4	0		433.2	0	420.5	0		580.9	0	563.8	0
A' Pb-F str.	494.0, **487.7**	463.4	94	451.5	79.5	493.3, **486.5**	462.6	92	450.5	78	493.8, **487.4**	463.3	95	451.3	81
A' C-Pb str.	440.2	410.6	50	400.7	48		376.4	40	367.6	38	427.7	398.4	47	388.8	44
A' CPbF bend		150.9	6	148.2	5		140.2	6	137.5	5		149.1	6	146.4	5
A" CH_3 tort		30.9	0	37.9	0		21.3	1	27.0	1		30.9	0	37.9	0

[a] Frequencies and infrared intensities are in cm^{-1} and km/mol. [b] Observed in an argon matrix, and the stronger one in an absorption set is bold. [c] Computed with B3LYP/6-311++G(3df,3pd). [d] Computed with BPW91/6-311++G(3df, 3pd). The SDD core potential and basis set are used for Pb. CH_3-PbF has a C_s structure, and the symmetry notations are based on the structure.

Table S3: Observed and Calculated Fundamental Frequencies of CH_2F-PbF Isotopomers in the ^{1}A' State[a]

Approximate Description	CH_2F-PbF					CD_2F-PbF				
	Obs[b]	B3LYP[c]		BPW91[d]		Obs[b]	B3LYP[c]		BPW91[d]	
		Freq	Int[d]	Freq	int		Freq	Int[d]	Freq	int
A" CH_2 as str.		3085.4	28	3022.7	27		2289.2	18	2242.6	17
A' CH_2 s str.		3025.8	29	2959.9	29		2191.3	16	2143.1	17
A' CH_2 scis.		1452.6	1	1404.7	1		1071.4	30	1037.4	31
A' CH_2 wag		1226.8	18	1182.0	18		937.1	53	911.3	8
A" CH_2 twist	1192.2	1213.3	2	1178.8	1		901.8	2	876.2	1
A' C-F str.	982.3	969.8	156	946.7	157	974.2	959.3	78	925.4	122
A" CH_2 rock		553.6	0	536.4	0		420.5	0	407.9	0
A' Pb-F str.	498.1, **492.3**	469.6	93	457.1	79	497.8, **491.8**	469.1	96	456.6	83
A' C-Pb str.		446.5	27	431.3	22		409.1	23	395.8	19
A' FCPb bend		196.6	2	189.1	2		194.9	3	187.4	2
A' CPbF bend		89.3	13	86.3	11		88.6	13	85.6	11
A" CH_2F tort.		51.4	10	47.4	9		45.9	9	42.4	8

[a] Frequencies and infrared intensities are in cm^{-1} and km/mol. [b] Observed in an argon matrix, and the stronger one in an absorption set is bold. [c] Computed with B3LYP/6-311++G(3df,3pd). [d] Computed with BPW91/6-311++G(3df, 3pd). The SDD core potential and basis set are used for Pb. CH_2F-PbF has a C_s structure.

Table S4: Observed and Calculated Fundamental Frequencies of CH_2F-PbCl Isotopomers in the $^1A'$ State[a]

Approximate Description	CH_2F-PbCl				
	Obs[b]	B3LYP[c]		BPW91[d]	
		Freq	Int	Freq	int
A" CH_2 as str.		3092.7	22	3029.2	22
A' CH_2 s str.		3030.8	23	2964.6	23
A' CH_2 scis.		1450.5	1	1401.9	0
A' CH_2 wag	1192.9	1224.8	16	1178.9	1
A" CH_2 twist		1215.2	1	1177.9	16
A' C-F str.	987.8	972.2	169	950.0	173
A" CH_2 rock		561.3	0	540.2	0
A' C-Pb str.		449.2	12	433.7	9
A' Pb-Cl str.		279.6	56	281.2	48
A' FCPb bend		191.9	6	184.8	5
A' CPbCl bend		70.8	6	68.2	5
A" CH_2F tort.		58.1	7	50.1	6

[a] Frequencies and infrared intensities are in cm^{-1} and km/mol. [b] Observed in an argon matrix. [c] Computed with B3LYP/6-311++G(3df,3pd). [d] Computed with BPW91/6-311++G(3df, 3pd). The SDD core potential and basis set are used for Pb. CH_2F-PbCl has a C_s structure.

Table S5: Observed and Calculated Fundamental Frequencies of CH_2Cl-PbF Isotopomers in the ^1A State[a]

Approximate Description	CH_2Cl-PbF				
	Obs[b]	B3LYP[c]		BPW91[d]	
		Freq	Int	Freq	int
CH_2 as str.		3181.6	3	3132.0	2
CH_2 s str.		3095.0	14	3039.0	13
CH_2 scis.		1418.4	2	1367.0	2
CH_2 wag		1096.3	4	1043.1	3
CH_2 twist		1077.7	0	1041.9	0
C-Cl str.	621.9	621.8	20	614.8	16
CH_2 rock		605.9	7	584.6	7
Pb-F str.	495.0	468.2	96	454.0	83
C-Pb str.		411.5	37	400.8	30
CPbF bend		145.8	4	142.6	4
PbCF bend		97.9	12	105.3	13
CH_2F twist		45.5	3	54.3	3

[a] Frequencies and infrared intensities are in cm^{-1} and km/mol. [b] Observed in an argon matrix. [c] Computed with B3LYP/6-311++G(3df,3pd). [d] Computed with BPW91/6-311++G(3df, 3pd). The SDD core potential and basis set are used for Pb. CH_2Cl-PbF has a C_1 structure.

Table S6: Observed and Calculated Fundamental Frequencies of CH_2Cl-PbCl Isotopomers in the Ground ^1A State[a]

Approximate Description	CH_2Cl-PbCl					CD_2Cl-PbCl					$^{13}CH_2Cl$-PbCl				
	Obs[b]	B3LYP[c]		BPW91[d]		Obs[b]	B3LYP[c]		BPW91[d]		Obs[b]	B3LYP[c]		BPW91[d]	
		Freq	Int	Freq	Int		Freq	Int	Freq	Int		Freq	Int	Freq	Int
CH_2 as str.		3184.6	2	3134.5	2		2367.8	1	2331.3	1		3171.9	2	3121.9	2
CH_2 s str.		3096.6	13	3040.5	12		2242.0	5	2200.6	5		3091.1	13	3035.2	12
CH_2 scis.		1421.0	2	1371.0	2		1040.4	3	1004.1	2		1417.4	2	1367.6	2
CH_2 wag		1099.2	6	1045.3	4		840.3	3	798.9	1		1093.3	6	1040.5	2
CH_2 twist		1077.8	0	1041.0	0		781.2	0	756.0	0		1076.3	0	1038.5	2
C-Cl str.	632.1, **626.5**	627.9	20	619.5	17	622.0, **617.5**	615.4	18	608.0	15	615.5, **610.7**	610.7	19	602.9	16
CH_2 rock		620.4	6	596.8	6		477.6	4	457.4	4		616.0	7	592.4	6
C-Pb str.		415.3	26	404.9	20		379.2	22	369.9	18		402.9	24	392.7	19
Pb-Cl str.		277.5	59	277.5	51		277.4	59	277.4	51		277.5	59	277.5	51
CPbCl bend		129.9	1	126.0	1		117.4	1	113.9	2		127.6	1	123.8	1
PbCCl bend		94.0	10	101.3	12		93.0	10	99.9	11		93.6	10	100.9	12
Pb-Cl tort		37.9	2	42.5	1		37.2	2	42.0	1		37.8	2	42.5	1

[a] Frequencies and infrared intensities are in cm^{-1} and km/mol. [b] Observed in an argon matrix, and the stronger one in an absorption set is bold. [c] Computed with B3LYP/6-311++G(3df,3pd). [d] Computed with BPW91/6-311++G(3df, 3pd). The SDD core potential and basis set are used for Pb. CH_2Cl-PbCl has a C_1 structure, and the symmetry notations are based on the structure.

Table S7: Observed and Calculated Fundamental Frequencies of CHF_2-PbF Isotopomers in the ^{1}A' State[a]

Approximate Description	CHF_2-PbF					CDF_2-PbF				
	Obs[b]	B3LYP[c]		BPW91[d]		Obs[b]	B3LYP[c]		BPW91[d]	
		Freq	Int	Freq	Int		Freq	Int	Freq	Int
A' C-H str.		3060.8	34	3022.7	27		2251.8	23	2242.6	17
A" C-H oop bend		1345.4	2	2959.9	29		971.2	18	2143.1	17
A' C-H ip bend	1241.8	1247.2	82	1404.7	1	1027.1, 1025.0	934.1	120	1037.4	31
A' CF_2 s str.	1061.7, **1050.3**, 1043.9	1036.8	211	1182.0	18	1045.4, **1040.8**	1040.0	237	925.4	122
A" CF_2 as str.	998.7, **996.9**	965.9	222	1178.8	1	938.8	1013.9	104	911.3	8
A' CF_2 scis.		515.5	3	946.7	157		510.6	2	876.2	1
A' CHF_2 rock		495.8	7	536.4	0		444.3	13	456.6	83
A' Pb-F str.	499.1	474.9	98	457.1	79	498.9	475.4	95	407.9	0
A' C-Pb str.		175.6	7	431.3	22		175.4	7	395.8	19
A" CHF_2 rock		115.0	0	189.1	2		114.9	0	187.4	2
A' CPbF bend		94.4	14	86.3	11		93.7	14	85.6	11
A" Pb-F tort.		22.2	8	47.4	9		22.0	8	42.4	8

[a] Frequencies and infrared intensities are in cm^{-1} and km/mol. [b] Observed in an argon matrix, and the stronger one in an absorption set is bold. [c] Computed with B3LYP/6-311++G(3df,3pd). [d] Computed with BPW91/6-311++G(3df, 3pd). The SDD core potential and basis set are used for Pb. CH_2F-PbF has a C_s structure, and the symmetry notations are based on the structure.

Table S8: Observed and Calculated Fundamental Frequencies of CF_3-PbF in the Ground ^{1}A' State[a]

Approximate Description	CF_3-PbF				
	Obs[b]	B3LYP[c]		BPW91[d]	
		Freq	Int	Freq	Int
A' CCl_3 s str.	1138.2, **1126.8**	1130.3	269	1077.9	279
A" CCl_3 as str.	**1037.4**, 1034.9	1045.4	266	994.2	259
A' CCl_3 as str.	948.4	1000.7	271	950.1	263
A' C-Pb str.		692.0	1	664.7	1
A' Pb-Cl str.		497.4	0	477.5	0
A' CCl_3 deform		495.8	3	476.3	32
A" CCl_3 deform	518.0	488.8	90	472.6	48
A' CPbCl bend		205.1	25	197.3	21
A' CCl_3 rock		168.3	6	160.7	4
A" CCl_3 rock		118.2	1	108.6	1
A' CPbCl bend		97.1	6	88.8	5
A" Pb-Cl tort		10.9	5	8.7	5

[a] Frequencies and infrared intensities are in cm^{-1} and km/mol. [b] Observed in an argon matrix, and the stronger one in an absorption set is bold. [c] Computed with B3LYP/6-311++G(3df,3pd). [d] Computed with BPW91/6-311++G(3df, 3pd). The SDD core potential and basis set are used for Pb. CF_3-PbF has a C_s structure, and the symmetry notations are based on the structure.

Table S9: Observed and Calculated Fundamental Frequencies of CF_3-PbCl in the Ground ^{1}A' State[a]

Approximate Description	CF_3-PbCl				
	Obs[b]	B3LYP[c]		BPW91[d]	
		Freq	Int	Freq	Int
A' CF3 s. str.	1073.8	1129.6	251	1076.1	261
A' CF3 as. str.	1041.5	1048.0	283	996.7	277
A" CF3 as. str.	1004.0	1005.2	262	955.2	255
A' CF3 bend		693.6	1	666.8	1
A" CF3 deform		499.5	0	479.7	0
A' CF3 deform		496.0	0	475.7	0
A' Pb-Cl str.		293.3	54	293.1	47
A' CF3 rock		202.0	17	195.8	15
A' C-Pb str.		168.0	7	161.7	6
A" CF3 rock		123.6	1	115.9	1
A' CPbCl bend		73.6	2	71.0	2
A" Pb-Cl tort		15.4	2	15.3	1

[a] Frequencies and infrared intensities are in cm^{-1} and km/mol. [b] Observed in an argon matrix. [c] Computed with B3LYP/6-311++G(3df,3pd). [d] Computed with BPW91/6-311++G(3df, 3pd). The SDD core potential and basis set are used for Pb. CF_2Cl-PbCl has a C_s structure, and the symmetry notations are based on the structure.

Table S10: Observed and Calculated Fundamental Frequencies of CF_2Cl-PbF in the Ground ^1A State[a]

Approximate Description	CF_2Cl-PbF				
	Obs[b]	B3LYP[c]		BPW91[d]	
		Freq	Int	Freq	Int
CF_2 s. str.	1063.9	1128.8	212	1108.9	233
CF_2 as. str.	1035.9, **1032.0**	1054.3	214	1038.1	221
C-Cl str.	711.1	674.9	129	624.9	50
CF_2 bend	629.4	592.8	41	559.7	68
Pb-F str.	477.3	485.7	94	468.0	83
C-Cl bend		344.5	1	314.0	1
CF_2Cl deform		338.7	27	282.0	40
C-Pb str.		198.2	27	189.7	25
CF_2Cl rock		166.1	4	157.8	1
CPbF bend		90.7	6	88.9	6
ClCPb bend		65.1	1	74.6	1
Pb-F tort		38.5	5	54.4	5

[a] Frequencies and infrared intensities are in cm^{-1} and km/mol. [b] Observed in an argon matrix, and the stronger one in an absorption set is bold. [c] Computed with B3LYP/6-311++G(3df,3pd). [d] Computed with BPW91/6-311++G(3df, 3pd). The SDD core potential and basis set are used for Pb. CF_2Cl-PbCl has a C_1 structure, and the symmetry notations are based on the structure.

Table S11: Observed and Calculated Fundamental Frequencies of CF_2Cl-PbCl in the Ground $^1A_2$ State[a]

Approximate Description	CF_2Cl-PbCl				
	Obs[b]	B3LYP[c]		BPW91[d]	
		Freq	Int	Freq	Int
CF_2 s str.	1109.6	1122.6	191	1100.8	216
CF_2 as str.	1021.9	1047.0	216	1032.4	224
C-Cl str.	707.9, **685.5**	686.9	144	631.3	66
CF_2 scis.	598.9, **596.9**	596.0	30	567.0	56
CF_2Cl bend		351.1	19	320.9	0
CF_2Cl deform		348.8	2	297.9	31
Pb-Cl str.		292.2	56	287.6	52
C-Pb str.		196.3	20	188.6	19
CF_2Cl rock		165.6	5	157.2	2
CPbCl str.		70.5	3	74.1	5
CF_2Cl rock		67.8	1	65.7	1
CF_2Cl tort.		32.1	2	42.8	1

[a] Frequencies and infrared intensities are in cm^{-1} and km/mol. [b] Observed in an argon matrix, and the stronger one in an absorption set is bold. [c] Computed with B3LYP/6-311++G(3df,3pd). [d] Computed with BPW91/6-311++G(3df, 3pd). The SDD core potential and basis set are used for Pb. CF_2Cl-PbCl has a C_1 structure, and the symmetry notations are based on the structure.

Table S12: Observed and Calculated Fundamental Frequencies of $CFCl_2$-PbCl in the Ground $^1A_2$ State[a]

Approximate Description	$CFCl_2$-PbCl				
	Obs[b]	B3LYP[c]		BPW91[d]	
		Freq	Int	Freq	Int
A' C-F str.	**1017.1**, 1011.5	1081.8	121	1055.3	131
A' CCl_2 s str.	673.2	711.6	62	706.5	126
A" CCl_2 as str.	654.7	666.2	106	601.5	131
A' CCl_2 wag.		443.7	12	427.6	13
A" $CFCl_2$ deform		352.2	4	330.3	8
A' Pb-Cl str.		289.9	59	288.1	51
A' CCl_2 scis.		271.9	0	257.8	1
A' FCPb bend		196.0	21	187.7	18
A' $CFCl_2$ rock		119.7	6	116.0	4
A' CPbCl bend		65.9	2	65.4	4
A" $CFCl_2$ rock		64.7	1	53.3	1
A" $CFCl_2$ tort.		6.0	2	26.0	1

[a] Frequencies and infrared intensities are in cm^{-1} and km/mol. [b] Observed in an argon matrix, and the stronger one in an absorption set is bold. [c] Computed with B3LYP/6-311++G(3df,3pd). [d] Computed with BPW91/6-311++G(3df, 3pd). The SDD core potential and basis set are used for Pb. $CFCl_2$-PbCl has a C_s structure, and the symmetry notations are based on the structure.

Table S13: Observed and Calculated Fundamental Frequencies of CCl_3-PbCl in the Ground ^{1}A' State[a]

Approximate Description	CCl_3-PbCl					$^{13}CCl_3$-PbCl				
	Obs[b]	B3LYP[c]		BPW91[d]		Obs[b]	B3LYP[c]		BPW91[d]	
		Freq	Int	Freq	Int		Freq	Int	Freq	Int
A' CCl_3 s str.	718.5	744.4	58	726.7	64	694.0	719.3	55	102.2	61
A' CCl_3 as str.	640.9	655.3	52	630.9	56	617.6	633.0	48	609.5	52
A" CCl_3 as str.	628.5	629.5	128	600.8	130	610.6	609.2	121	581.6	122
A' C-Pb str.		372.4	7	364.1	7		372.1	7	363.3	7
A' Pb-Cl str.		289.0	56	287.9	49		289.0	56	287.9	49
A' CCl_3 deform		260.1	0	250.9	0		259.6	0	250.3	0
A" CCl_3 deform		259.0	1	250.4	1		258.6	1	250.0	1
A' CPbCl bend		145.3	17	141.7	15		145.2	17	141.6	15
A' CCl_3 rock		116.3	3	110.0	2		116.1	3	109.8	2
A" CCl_3 rock		75.0	3	66.1	2		75.0	3	66.1	2
A' CPbCl bend		71.1	0	56.4	0		70.9	0	56.2	0
A" Pb-Cl tort		11.8	2	18.5	2		11.8	2	18.5	2

[a] Frequencies and infrared intensities are in cm^{-1} and km/mol. [b] Observed in an argon matrix. [c] Computed with B3LYP/6-311++G(3df,3pd). [d] Computed with BPW91/6-311++G(3df, 3pd). The SDD core potential and basis set are used for Pb. CCl_3-PbCl has a C_s structure, and the symmetry notations are based on the structure.

Table S14: Observed and Calculated Fundamental Frequencies of CCl_2-$PbCl_2$ in the Ground ^{1}A' State[a]

Approximate Description	CCl_2-$PbCl_2$					$^{13}CCl_2$-$PbCl_2$				
	Obs[b]	B3LYP[c]		BPW91[d]		Obs[b]	B3LYP[c]		BPW91[d]	
		Freq	Int	Freq	Int		Freq	Int	Freq	Int
A" CCl_2 as. str.	**874.7**, 872.5, 864.4	866.8	263	847.6	240	**847.4**, 845.4, 839.5	839.2	246	820.7	225
A' CCl_2 s. str.	covered	793.9	42	769.0	102	covered	769.8	41	745.5	96
A' CCl_2 scis		362.2	3	353.2	2		360.5	3	351.5	2
A' CCl_2Pb bend		276.2	21	282.6	14		272.6	35	275.3	21
A' $PbCl_2$ s. str.		267.8	18	265.3	22		261.7	4	262.9	15
A" $PbCl_2$ as. str.		251.7	70	249.8	57		251.7	70	249.8	57
A" CCl_2 rock.		105.8	0	106.0	0		105.3	0	105.5	0
A' C-Pb str.		93.2	6	96.7	1		92.9	6	96.3	1
A' $PbCl_2$ scis.		85.6	2	82.4	2		85.6	2	82.4	2
A' $PbCl_2$ wag		65.4	10	62.2	0		65.4	10	62.1	0
A" CCl_2 rock		62.8	0	59.8	8		62.8	0	59.8	8
A" CCl_2 tort.		18.1	1	24.1	1		19.1	1	24.1	1

[a] Frequencies and infrared intensities are in cm^{-1} and km/mol. [b] Observed in an argon matrix, and the strongest one in an absorption set is bold. [c] Computed with B3LYP/6-311++G(3df,3pd). [d] Computed with BPW91/6-311++G(3df, 3pd). CCl_2-$PbCl_2$ has a C_s structure, and the symmetry notations are based on the structure.

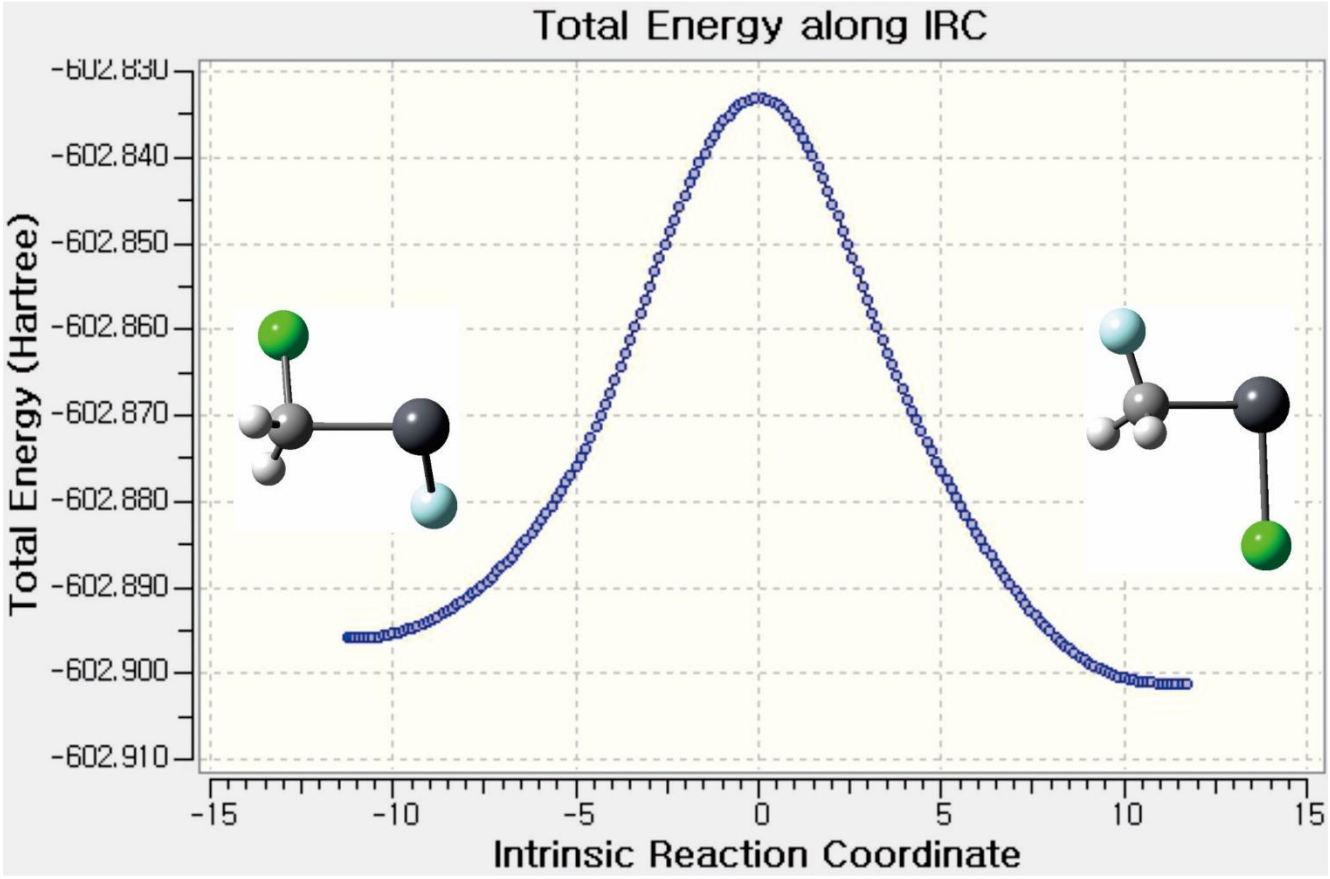

Figure S1. Interconversion between CH_2Cl-PbF and CH_2F-PbCl.

C_2H_5-PbH

C	-1.735811	-0.675445	0.119622
H	-1.864141	-1.499448	-0.584340
H	-1.825157	-1.113959	1.119762
C	-2.801671	0.400531	-0.086294
H	-3.814231	-0.002944	0.015656
H	-2.740734	0.849256	-1.080136
H	-2.695051	1.209983	0.636314
Pb	0.488542	0.006920	-0.012809
H	0.103728	1.639117	0.743111

$CH_3CH=PbH_2$

C	-1.562625	0.588979	-0.144183
H	-1.735985	1.635946	0.091003
C	-2.766602	-0.277071	0.017591
H	-3.515118	0.033016	-0.722265
H	-3.251216	-0.168478	0.993848
H	-2.563156	-1.334313	-0.148824
Pb	0.422368	-0.019174	0.020215
H	0.790052	-1.605973	-0.612606
H	1.616599	1.140641	-0.499232

$(CH_2)_2PbH_2$

Pb	0.000000	0.468560	0.000000
H	-1.244172	0.209857	1.318081
H	-1.244172	0.209857	-1.318081
C	-0.508455	-2.515904	0.000000
C	0.817660	-2.326792	0.000000
H	-1.067867	-2.603055	-0.920829
H	-1.067867	-2.603055	0.920829
H	1.384424	-2.289663	-0.920943
H	1.384424	-2.289663	0.920943

$CH_3C\text{-}PbH_3(T)$

C	-3.021699	0.132489	-0.000004
H	-3.192496	0.760884	-0.884924
H	-3.805302	-0.633872	0.000313
H	-3.192266	0.761404	0.884590
C	-1.692540	-0.484516	0.000004
Pb	0.433555	0.010096	0.000000
H	0.806316	0.936633	-1.427392
H	1.311962	-1.479789	0.001435
H	0.805723	0.939046	1.425993

CH_3-PbF

Pb	0.120598	-0.252536	0.000000
F	1.021078	1.623816	-0.000001
C	-2.005060	0.629605	-0.000030
H	-1.931884	1.715096	-0.002817
H	-2.559325	0.298167	-0.880343
H	-2.557150	0.302755	0.883357

CH_2F-PbH

Pb	-0.457634	-0.043343	0.000009
H	-0.963441	1.726054	-0.000982
C	1.777893	0.622899	0.000167
H	2.008436	1.223856	-0.882713
H	2.008394	1.223332	0.883424
F	2.645029	-0.484060	-0.000159

CH_2=PbHF

C	1.723376	0.960208	0.177734
H	2.645648	0.442830	-0.072193
H	1.650586	1.945517	-0.273273
Pb	0.010358	-0.192471	-0.023274
H	-0.653616	-1.577468	0.785511

F	-1.648027	1.023392	0.044671

$CH\text{-}PbH_2F$

C	-1.727173	1.290463	-0.000064
C	-2.631494	0.643592	-0.000008
Pb	-0.024352	-0.190667	0.000000
H	0.236019	-1.086722	-1.465388
H	0.235740	-1.085692	1.466053
F	1.613294	1.046748	-0.000030

$CH_2F\text{-}PbF$

Pb	0.327704	-0.258033	0.000015
F	1.352790	1.549152	-0.000149
C	-1.728594	0.850483	0.000295
H	-1.844196	1.480305	0.884443
H	-1.843457	1.480474	-0.883882
F	-2.776407	-0.094154	-0.000247

$CHF_2\text{-}PbH$

Pb	-0.646194	-0.000003	-0.011784
H	-0.310273	0.000193	1.780469
C	1.705327	-0.000010	-0.412243

H	2.030192	-0.000026	-1.455433
F	2.279773	1.110578	0.173019
F	2.279788	-1.110567	0.173061

CH_2=PbF_2

C	-2.109753	-0.000037	0.577039
H	-2.615222	0.889304	0.187821
H	-2.615189	-0.889421	0.187878
Pb	-0.043154	-0.000007	-0.127092
F	1.190354	1.538412	0.365749
F	1.190486	-1.538314	0.365763

CH-$PbHF_2$

C	1.320057	1.733632	0.503708
H	0.857000	1.941394	1.491390
Pb	-0.011539	0.007401	-0.200185
H	-0.420408	-0.585478	-1.765463
F	-1.801575	0.141473	0.782161
F	0.978158	-1.515320	0.736396

CH_2F-PbCl

Pb	-0.035404	-0.462576	0.000016

Cl	-1.998530	1.124820	-0.000092
C	1.489250	1.306141	0.000386
H	1.372136	1.933319	-0.884864
H	1.373002	1.933040	0.885926
F	2.799722	0.789562	-0.000347

CH_2Cl-PbF

Pb	-0.545908	-0.241965	-0.008445
F	-1.152309	1.732360	-0.220363
C	1.446583	0.362162	1.045524
H	1.515960	1.420266	1.272055
H	1.827815	-0.243967	1.860267
Cl	2.535997	0.052978	-0.395867

TS CH_2F-PbCl ↔ CH_2Cl-PbF

Pb	-0.383014	-0.375307	0.000080
F	-1.559362	1.665179	-0.001120
C	0.466257	1.621923	0.001411
H	0.669478	2.178680	-0.905550
H	0.668963	2.179152	0.908229
Cl	2.429730	0.099951	-0.000448

CH_2=PbFCl

C	-1.763109	-1.306740	0.669557
H	-2.752945	-0.901772	0.441066
H	-1.672693	-2.307573	0.239234
Pb	-0.228961	-0.003041	-0.144884
F	-0.373109	1.950862	0.422003
Cl	2.184534	-0.368152	0.199108

CH-PbHFCl

C	1.480282	-0.757426	0.354547
H	1.731337	-1.807633	0.189919
Pb	-0.638933	-0.163697	-0.046755
H	-1.621388	-0.518294	1.406733
F	-0.503816	1.898329	0.132280
Cl	2.819718	0.188748	-0.063560

CH_2Cl-PbCl

Pb	-0.320223	-0.510739	-0.017917
Cl	-1.743689	1.576912	-0.075803
C	1.472497	0.528346	1.058123
H	1.279189	1.548051	1.369973
H	2.003906	-0.027574	1.823029

Cl	2.575466	0.610738	-0.399051

CH_2=$PbCl_2$

C	-0.001256	2.215728	0.787179
H	0.893209	2.784029	0.522426
H	-0.896643	2.782356	0.521803
Pb	-0.000169	0.275184	-0.166551
Cl	1.932301	-1.217512	0.232041
Cl	-1.930840	-1.219304	0.232069

CH-$PbHCl_2$

C	-1.633832	-0.676471	0.396217
H	-2.030751	-1.692175	0.338228
Pb	0.538998	-0.430770	-0.048405
H	1.408476	-0.959474	1.420007
Cl	-2.841142	0.407408	-0.077236
Cl	0.854521	2.065157	0.067452

CHF_2-PbF

Pb	0.530749	-0.244323	0.000235
F	1.260161	1.693081	-0.001939
C	-1.719816	0.517819	-0.001006

H	-1.881824	1.596888	-0.002930
F	-2.370756	0.003059	-1.108302
F	-2.369480	0.007271	1.109094

CF_3-PbH

Pb	0.187434	0.783229	0.000000
H	-1.579142	1.249820	0.000000
C	-0.359621	-1.554800	0.000000
F	0.187434	-2.169296	1.088782
F	-1.667397	-1.899834	0.000000
F	0.187434	-2.169296	-1.088782

CH-PbF_3

C	-2.362457	-0.160749	0.001897
H	-2.620649	0.922552	-0.000419
Pb	-0.048386	-0.003236	0.000069
F	0.772569	-0.904764	1.598822
F	0.764559	1.847178	-0.002552
F	0.769877	-0.908268	-1.598117

$CHCl_2$-PbCl

Pb	0.629357	-0.085992	-0.495612

Cl	2.109577	0.252589	1.512536
C	-1.380992	0.112833	0.712011
H	-1.297355	0.278788	1.778480
Cl	-2.274708	1.521594	0.032010
Cl	-2.306868	-1.415619	0.490140

CCl_3-PbH

Pb	-1.191978	0.142477	0.000000
H	-1.546792	-1.655487	0.000000
C	1.183808	-0.186263	0.000000
Cl	1.807572	0.665949	1.470387
Cl	1.807572	-1.856019	0.000000
Cl	1.807572	0.665949	-1.470387

CH-$PbCl_3$

C	-1.538327	-0.256940	-0.528477
H	-1.931212	-0.866173	-1.334127
Pb	0.809872	-0.391306	-0.190321
Cl	1.080226	1.891946	0.792091
Cl	-1.981464	-1.173372	1.000861
Cl	-2.348663	1.310537	-0.609932

CF_3-PbF

Pb	0.720067	-0.227957	-0.000013
F	1.130711	1.785282	-0.000030
C	-1.669154	0.075195	-0.000063
F	-2.144760	1.331108	-0.001785
F	-2.217169	-0.546387	-1.088372
F	-2.216623	-0.543191	1.090346

CF_2-PbF_2

C	-2.096529	0.000077	-0.307053
F	-2.826319	1.032582	-0.089233
F	-2.826587	-1.032431	-0.090068
Pb	0.736916	-0.000151	-0.193108
F	0.168582	1.550317	1.070960
F	0.167890	-1.549147	1.072477

CF-PbF_3

C	-2.194786	-0.960635	0.000217
F	-2.929812	0.045255	0.000023
Pb	0.180208	-0.038991	0.000012
F	1.328717	-0.524685	1.602381
F	0.093506	2.001063	-0.000807

F	1.328885	-0.525958	-1.601846

CF_3-PbCl

Pb	0.698176	0.254877	0.000000
Cl	-0.866567	2.196259	0.000000
C	-1.024576	-1.428974	0.000000
F	-2.308125	-1.039637	0.000000
F	-0.866567	-2.239210	1.089513
F	-0.866567	-2.239210	-1.089513

CF_2Cl-PbF

Pb	0.840859	-0.206801	0.112641
F	1.300844	1.500645	-0.939416
C	-1.473904	0.367450	0.358948
F	-1.921301	1.597117	0.094420
F	-2.092558	-0.037119	1.491101
Cl	-2.099405	-0.752521	-1.012069

CF-PbF_2Cl

C	2.488764	0.084371	-0.000514
F	2.730551	1.310195	-0.000070
Pb	-0.029303	-0.201429	-0.000027

F	-0.523629	-1.362669	1.595540
F	-0.524552	-1.363129	-1.594955
Cl	-1.627711	1.691258	0.000042

$CCl\text{-}PbF_3$

C	-1.808534	0.483415	-1.048752
Cl	-2.964702	-0.006056	0.012356
Pb	0.392131	0.019220	-0.042238
F	1.571617	1.627253	0.325708
F	1.598007	-1.266286	-1.044364
F	0.063308	-0.846922	1.779322

$CF_2Cl\text{-}PbCl$

Pb	0.662825	-0.525024	-0.020932
Cl	1.727633	1.725490	0.151889
C	-1.537341	0.312600	-0.469138
F	-1.742833	1.583124	-0.826790
F	-2.289201	-0.450251	-1.298399
Cl	-2.247592	0.096894	1.239755

$CFCl_2\text{-}PbF$

Pb	0.962056	0.000353	-0.261916

F	1.711046	-0.002178	1.655656
C	-1.339562	-0.000398	0.403583
F	-1.639097	-0.001630	1.712108
Cl	-2.102799	-1.478231	-0.332373
Cl	-2.103012	1.478684	-0.329642

CF-$PbFCl_2$

C	-1.908040	-1.621983	-0.463758
F	-2.886815	-0.875433	-0.681409
Pb	0.039144	-0.096795	0.085271
F	0.147779	-0.298884	2.114759
Cl	-0.368215	2.326294	-0.292958
Cl	2.302909	-0.665239	-0.713504

CCl-PbF_2Cl

C	1.873376	-0.514646	-1.152712
C	3.057994	-0.487266	-0.015349
Pb	-0.237211	0.119065	-0.038334
F	-0.711179	2.020456	-0.588633
F	0.291949	0.309166	1.932031
Cl	-2.353048	-1.138736	-0.104119

$CFCl_2$-PbCl

Pb	0.764510	-0.535994	0.018673
Cl	2.095349	1.578051	-0.071278
C	-1.387234	0.515073	-0.034687
F	-1.463405	1.852546	-0.122500
Cl	-2.293339	-0.176535	-1.445346
Cl	-2.225291	0.021316	1.503652

CCl_3-PbF

Pb	0.430349	1.030051	0.000000
F	-1.438328	1.889825	0.000000
C	-0.321656	-1.243257	0.000000
Cl	-2.061508	-1.546276	0.000000
Cl	0.430349	-1.991952	1.470413
Cl	0.430349	-1.991952	-1.470413

CF-$PbCl_3$

C	1.856792	-0.001057	-1.778478
F	2.918786	0.000477	-1.117065
Pb	-0.022873	-0.000077	-0.085465
Cl	0.888727	-0.009124	2.233605
Cl	-1.495127	-1.979760	-0.306897

Cl	-1.483848	1.989378	-0.295377

CCl-$PbFCl_2$

C	1.961839	0.000140	-1.227566
Cl	3.168897	-0.000294	-0.113057
Pb	-0.180676	-0.000058	-0.004875
F	0.443636	0.000326	1.950246
Cl	-1.612659	-2.002863	-0.231269
Cl	-1.612024	2.003213	-0.231384

CCl_3-$PbCl$				Mulliken Charge	Natural Charge
Pb	0.544917	0.904696	0.000000	0.784842	1.30647
Cl	-1.685246	2.031190	0.000000	-0.547950	-0.61632
C	-0.223353	-1.368197	0.000000	0.992882	-0.71656
Cl	-1.954179	-1.712918	0.000000	-0.225149	0.01913
Cl	0.544917	-2.099602	1.470454	-0.502312	-0.01185
Cl	0.544917	-2.099602	-1.470454	-0.502312	0.01913

CCl_2-$PbCl_2$				Mulliken Charge	Natural Charge
Pb	-0.896711	-0.000538	-0.471252	0.028849	-0.28620
Cl	-0.823586	1.963299	1.167489	0.113623	0.19527
Cl	-0.821631	-1.962239	1.169833	0.113623	0.19527

C	1.775379	0.000445	-0.176946	0.851681	1.19392
Cl	2.672523	-1.409656	-0.001654	-0.553888	-0.64913
Cl	2.671402	1.411035	-0.000119	-0.553888	-0.64913

CCl-$PbCl_3$

C	1.787663	0.002232	-1.512148
Cl	3.125858	0.000382	-0.555875
Pb	-0.206943	0.000052	-0.077229
Cl	0.528095	-0.004613	2.310576
Cl	-1.644642	-1.983298	-0.427627
Cl	-1.642056	1.986490	-0.420859