Supporting information for

Revisiting a (001)-oriented Layered Lead Chloride Templated by 1,2,4-Triazolium: Structural Phase Transitions, Lattice Dynamics and Broadband Photoluminescence

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Table S1. The definitions of local vibrational coordinates for 1,2,4-triazolium cation.

Internal coordinate Label	Atom numbers	Assignment	Bond (Angs.)/ Angle (Deg.)
s1	1 7	νNH	1.022242
s2	2 8	νNH'	1.022652
s3	4 6	νCH	1.087192
s4	5 9	νCH'	1.087008
s5	3 5	νNC	1.313869
s6	2 4	νNC'	1.331561
s7	1 4	νNC''	1.345646
s8	3 2	νNN	1.359328
s9	5 3 2	δCNN	103.91
s10	7 1 5	δHNC	127.08
s11	8 2 3	δHNN	119.34
s12	6 4 2	δHCN	127.56
s13	9 5 3	δHCN'	125.05
s14	1 4 2	δNCN	105.2
s15	3 2 4	δNNC	112.97
s16	7 1 5 3	τHNCN	-180
s17	8 2 3 5	τHNNC	-180
s18	6 4 2 3	τHCNN	-180
s19	9 5 3 2	τHCNN'	-180
s20	5 3 2 4	τCNN)	0
s21	1 4 2 3	τNCN)	0

Table S2. The crystallographic data for Tz_2PbCl_4 ($C_4H_6Cl_4N_6Pb$) in phases I and II.

Phase		**I**	**I**	**II**	**II**
Temperature (K)		390	370	360	340
Formula weight		489.15	489.15	489.15	489.15
Wavelength (Å)		0.71073	0.71073	0.71073	0.71073
Crystal system		Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic
Space group		*Fmmm*	*Fmmm*	*Cmcm*	*Cmcm*
Unit cell dimensions (Å,°)	*a*	7.6009(7)	7.5639(2)	8.2929(2)	8.2959(15)
	b	8.3017(6)	8.2984(2)	7.5535(2)	7.4918(15)
	c	21.798(2)	21.7768(7)	21.7496(7)	21.829(6)
	β	90	90	90	90
Volume ($Å^3$)		1375.4(2)	1366.89(7)	1362.40(7)	1356.7(5)
Z/Z'		4/1	4/1	4/1	4/1
Calculated density (gcm^{-3})		2.362	2.377	2.385	2.395
Absorption coefficient (mm^{-1})		13.029	13.104	13.148	13.203
F(000)		896	896	896	896
Crystal size (mm)		0.616 × 0.26 × 0.14	0.62 × 0.26 × 0.14	0.616 × 0.26 × 0.14	0.56 × 0.18 × 0.12
Θ-range for data collection (°)		7.478 to 58.026	7.486 to 58.018	7.494 to 58.146	7.328 to 57.778
Min/max indices: *h, k, l*		-10 ≤ h ≤ 10, -10 ≤ k ≤ 11, -28 ≤ l ≤ 29	-10 ≤ h ≤ 10, -10 ≤ k ≤ 11, -28 ≤ l ≤ 29	-10 ≤ h ≤ 10, -10 ≤ k ≤ 11, -28 ≤ l ≤ 29	-11 ≤ h ≤ 10, -10 ≤ k ≤ 10, -29 ≤ l ≤ 27
Reflect. Collected/unique		6239/513	5515/308	11518/957	7079/908
Rint/ Completeness (%)		0.0767/96.7	0.0655/92.3	0.0598/92.5	0.0511/94.9
Data/restrains/parameters		513/15/30	515/27/30	957/0/43	908/0/43
Goodness-of-fit on F2		1.012	1.071	1.116	1.192
Final R1/wR2 (I>2δ1)		0.0258/0.0552	0.0222/0.0486	0.0233/0.0452	0.0296/0.0631
R1/wR2 (all data)		0.0260/0.0553	0.0222/0.0486	0.0369/0.0496	0.0377/0.0687

Table S3. The crystallographic data for Tz_2PbCl_4 ($C_4H_6Cl_4N_6Pb$) in phase III.

Phase		**III**	**III**	**III**
Temperature (K)		320	300	280
Formula weight		489.15	489.15	489.15
Wavelength (Å)		0.71073	0.71073	0.71073
Crystal system		Orthorhombic	Orthorhombic	Orthorhombic
Space group		*Pnma*	*Pnma*	*Pnma*
Unit cell dimensions (Å,°)	*a*	7.5195(2)	7.4929(3)	7.4798(4)
	b	21.5921(7)	21.5667(10)	21.5667(13)
	c	8.3020(2)	8.3106(4)	8.3086(4)
	β	90	90	90
Volume (Å^3)		1347.93(7)	1342.97(10)	1340.30(13)
Z/*Z'*		4/1	4/1	4/1
Calculated density (gcm^{-3})		2.41	2.419	2.424
Absorption coefficient (mm^{-1})		13.289	13.338	13.364
F(000)		896	896	896
Crystal size (mm)		0.616 × 0.261 × 0.144	0.555 × 0.15 × 0.123	0.56 × 0.18 × 0.12
Θ-range for data collection (°)		7.314 to 58.32	7.322 to 57.906	5.254 to 57.94
Min/max indices: h, k, l		-10 ≤ h ≤ 10, -28 ≤ k ≤ 29, -11 ≤ l ≤ 10	-10 ≤ h ≤ 10, -27 ≤ k ≤ 28, -11 ≤ l ≤ 10	-9 ≤ h ≤ 10, -28 ≤ k ≤ 27, -10 ≤ l ≤ 11
Reflect. Collected/unique		22255/1768	13880/1675	13755/1662
R_{int}/ Completeness (%)		0.0615/97.8	0.0465/97.4	0.0396/95.8
Data/restrains/parameters		1768/0/78	1675/0/78	1662/0/78
Goodness-of-fit on F^2		1.116	1.106	1.132
Final R_1/wR_2 (I>2δ_1)		0.0266/0.0460	0.0275/0.0618	0.0325/0.0546
R_1/wR^2 (all data)		0.0496/0.0512	0.0382/0.0668	0.0325/0.0575

Table S4. The crystallographic data for Tz_2PbCl_4 ($C_4H_6Cl_4N_6Pb$) in phase IV.

Phase		IV	IV	IV	IV	IV	IV	IV
Temperature (K)		250	220	200	180	150	130	100
Formula weight		487.14	487.14	487.14	487.14	487.14	487.14	487.14
Wavelength (Å)		0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal system		Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group		$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/c$
Unit cell dimensions (Å,°)	a	21.4566(15)	21.4831(12)	21.4212(18)	21.4424(18)	21.423(2)	21.429(2)	21.419(2)
	b	8.3029(3)	8.3057(3)	8.2997(3)	8.2994(3)	8.3075(4)	8.3075(4)	8.3049(4)
	c	7.4446(3)	7.4695(3)	7.4042(3)	7.4252(4)	7.3587(4)	7.3768(4)	7.3363(4)
	β	90.036(4)	90.036(4)	90.020(5)	90.093(5)	90.112(6)	90.111(6)	90.149(6)
Volume ($Å^3$)		1332.80(10)	1326.27(12)	1321.38(14)	1316.39(13)	1313.21(17)	1309.63(16)	1305.01(16)
Z/Z'		4/1	4/1	4/1	4/1	4/1	4/1	4/1
Calculated density (gcm^{-3})		2.438	2.45	2.459	2.468	2.474	2.481	2.49
Absorption coefficient (mm^{-1})		13.44	13.506	13.556	13.607	13.64	13.677	13.726
F(000)		896	896	896	896	896	896	896
Crystal size (mm)		0.56 × 0.18 × 0.12	0.56 × 0.18 × 0.12	0.555 × 0.179 × 0.122	0.56 × 0.18 × 0.12	0.56 × 0.18 × 0.12	0.555 × 0.179 × 0.122	0.56 × 0.18 × 0.12
Θ-range for data collection (°)		5.258 to 58.06	5.26 to 58.108	5.264 to 57.84	5.264 to 57.944	5.264 to 57.84	5.26 to 58.028	5.26 to 57.604

Min/max indices: h, k, l	$-28 \le h \le 27$, $-11 \le k \le 10$, $-10 \le l \le 9$	$-28 \le h \le 26$, $-11 \le k \le 10$, $-10 \le l \le 9$	$-28 \le h \le 26$, $-11 \le k \le 10$, $-10 \le l \le 9$	$-28 \le h \le 26$, $-11 \le k \le 10$, $-10 \le l \le 9$	$-26 \le h \le 28$, $-11 \le k \le 10$, $-9 \le l \le 9$	$-28 \le h \le 26$, $-11 \le k \le 10$, $-9 \le l \le 9$	$-28 \le h \le 26$, $-11 \le k \le 10$, $-9 \le l \le 9$
Reflect. Collected/unique	14644/3182	14514/3158	14455/3145	14257/3117	14206/3100	14134/3091	14033/3071
Rint/ Completeness (%)	0.0431/99.8	0.0417/99.8	0.0321/99.3	0.0380/99.2	0.0379/99.3	0.0376/99.2	0.0374/99.2
Data/restrains/parameters	3182/0/138	3158/0/78	3145/2/146	3117/0/138	3100/0/138	3091/0/138	3071/10/138
Goodness-of-fit on F^2	1.252	1.2	1.207	1.209	1.24	1.279	1.267
Final R_1/wR_2 ($I>2\delta_1$)	0.354/0.0849	0.0419/0.0935	0.0442/0.0996	0.0492/0.1064	0.0549/0.1152	0.0583/0.1163	0.0628/0.1204
R_1/wR^2 (all data)	0.0500/0.0906	0.0571/0.1007	0.0595/0.1069	0.0645/0.1150	0.0700/0.1245	0.0721/0.1241	0.0770/0.1286

Table S5. Selected hydrogen-bond parameters at various temperatures for phases I, II and III: hydrogen bond lengths (Å) and angles for normalized H-bond lengths (N-H =1.015 Å). A and B indicates two symmetry independent Tz^+ cations.

Temp.(K)		D···A (Å)	H···A (Å)	*D*—H···*A* (°)	D···A (Å)	H···A (Å)	*D*—H···*A* (°)
Phase I		N1-Cl2	H···Cl2	N1-H···Cl2			
390		3.151	2.113	165.00			
370		3.141	2.303	164.54			
Phase II		N1-Cl2	H···Cl2	N1-H···Cl2			
360		3.143	2.305	164.71			
340		3.140	2.304	164.25(5)			
Phase III		N2-Cl3	H···Cl3	N2-H···Cl3	N1-Cl3	H···Cl3	N1-H···Cl3
320		3.163(5)	2.255(5)	148.17(3)	3.145(5)	2.132(5)	175.54(1)
300		3.172(5)	2.272(5)	146.96(4)	3.143(5)	2.129(5)	176.19(1)
280		3.169(4)	2.270(4)	146.95(5)	3.136(4)	2.124(4)	174.57(4)
Phase IV		N2-Cl4/Cl3	H···Cl4/Cl3	N2-H···Cl4/Cl3	N1-Cl4/Cl3	H···Cl4/Cl3	N1-H···Cl4/Cl3
250	A	3.171(6)	2.276(6)	146.46(6)	3.170(6)	2.275(6)	173.30(2)
	B	3.140(6)	2.129(6)	146.26(4)	3.144(6)	2.134(6)	174.27(3)
220	A	3.171(6)	2.276(6)	146.45(5)	3.144(6)	2.134(6)	173.30(2)
	B	3.170(6)	2.275(6)	146.26(4)	3.140(6)	2.129(6)	174.27(3)
200	A	3.168(7)	2.205(7)	157.75(5)	3.145(7)	2.135(7)	173.01(1)
	B	3.132(7)	2.122(7)	157.38(2)	3.176(7)	2.215(7)	173.04(4)
180	A	3.176(8)	2.286(8)	145.63(10)	3.135(8)	2.126(8)	172.62(2)
	B	3.180(8)	2.299(8)	144.50(1)	3.134(8)	2.124(8)	173.18(2)
150	A	3.180(9)	2.297(9)	144.63(3)	3.144(10)	2.137(10)	171.25(5)
	B	3.183(9)	2.298(9)	145.09(1)	3.135(9)	2.127(9)	171.80(1)
130	A	3.185(5)	2.303(5)	144.62(2)	3.143(3)	2.136(3)	171.23(3)
	B	3.135(4)	2.303(4)	144.75(5)	3.146(5)	2.134(5)	171.26(4)
100	A	3.178(7)	2.296(7)	144.57(3)	3.146(7)	2.141(7)	170.06(3)
	B	3.180(8)	2.297(8)	144.74(5)	3.140(8)	2.134(8)	170.36(4)

Table S6. List of Pb-Cl-Pb angles (˚).

	Pb-Cl1-Pb	Pb-Cl2-Pb
390	180	-
370	180	-
360	179.7(1)	-
340	179.85(1)	-
320	173.3(1)	159.89(1)
300	172.76(1)	157.86(1)
280	172.29(2)	155.95(1)
250	172.01(6)	154.33(7)
220	171.63(7)	152.47(9)
200	171.37(8)	151.24(9)
180	171.1(1)	150.0(1)
150	170.9(1)	148.4(1)
130	170.8(1)	147.4(1)
100	170.7(1)	146.1(1)

Table S7. The bond length distortions of the individual $PbCl_6$ octahedra in phases I, II, III, and IV at different temperatures.

	Phase I	
Bonds (Å)	390 K	370 K
Pb1-Cl1	2.814(1)	2.807(1)
Pb1-Cl1'	2.814(1)	2.807(1)
Pb1-Cl1''	2.814(1)	2.807(1)
Pb1-Cl1'''	2.814(1)	2.807(1)
Pb1-Cl2	2.859(1)	2.855(1)
Pb1-Cl2''	2.859(1)	2.855(1)
d(Å)	2.8291	2.8231
Δd	1.82910	1.82310

i = 1-x,-y,z; ii = 1-x,y,-z; iii = x,-y,-z

	Phase II	
Bonds (Å)	360 K	340 K
Pb1-Cl1	2.806(1)	2.791(1)
Pb1-Cl1'	2.806(1)	2.791(1)
Pb1-Cl1''	2.803(1)	2.798(1)
Pb1-Cl1'''	2.803(1)	2.798(1)
Pb1-Cl2	2.857(1)	2.868(1)
Pb1-Cl2'	2.857(1)	2.868(1)
d(Å)	2.822	2.819
Δd	0.000614	0.001209

i = 1-x,y,0.5-z; ii = -0.5+x,-0.5+y,z; iii = 1.5-x,-0.5+y,0.5-z

	Phase III		
Bonds (Å)	320 K	300 K	280 K
Pb1-Cl1	2.843(1)	2.857(1)	2.851(1)
Pb1-Cl1'	2.793(1)	2.793(1)	2.794(1)
Pb1-Cl2	2.853(1)	2.857(1)	2.859(1)
Pb1-C2''	2.809(1)	2.809(1)	2.813(1)
Pb1-Cl3	2.861(1)	2.861(1)	2.864(1)
Pb1-Cl3''	2.861(1)	2.861(1)	2.864(1)
d(Å)	2.8368	2.8398	2.8409
Δd	1.83677	1.83977	1.84093

i = x,0.5-y,z; ii = -0.5+x,0.5-y,0.5-z

	Phase IV						
Bonds (Å)	250 K	220 K	200 K	180 K	150 K	130 K	100 K
Pb1-Cl1	2.793(2)	2.792(2)	2.792(2)	2.793(3)	2.793(3)	2.794(2)	2.793(2)
Pb1-Cl2	2.863(2)	2.867(2)	2.869(2)	2.871(2)	2.873(2)	2.873(2)	2.875(2)
Pb1-Cl3	2.859(2)	2.857(3)	2.852(2)	2.852(3)	2.846(4)	2.844(4)	2.846(4)
Pb1-C1'	2.858(2)	2.862(2)	2.864(2)	2.865(2)	2.870(2)	2.872(2)	2.875(3)
Pb1-Cl2''	2.811(2)	2.809(2)	2.806(2)	2.806(2)	2.806(3)	2.807(3)	2.805(3)
Pb1-Cl4	2.857(2)	2.854(3)	2.851(2)	2.846(2)	2.846(4)	2.848(4)	2.844(4)
d_{mean} (Å)	2.8404	2.8404	2.8392	2.8391	2.8393	2.8400	2.8400
Δd	1.84037	1.84040	1.83920	1.83907	1.83930	1.83995	1.83997

i = x,0.5-y,0.5-z; ii = x,1.5-y,0.5+z

Table S8. Bond angle variance of the individual $PbCl_6$ octahedra in phase **I** at different temperature.

Bond Angles (°)	390 K	370 K
Cl1-Pb1-Cl2	90.00(1)	90.00(1)
Cl1-Pb1-Cl1''	84.95(1)	84.70(1)
Cl1-Pb1-Cl1'''	95.05(1)	95.30(1)
Cl1-Pb1-Cl2''	90.00(1)	90.00(1)
Cl1'-Pb1-Cl2	90.00(1)	90.00(1)
Cl1'-Pb1-Cl1''	95.05(1)	95.30(1)
Cl1'-Pb1-Cl2''	90.00(1)	90.00(1)
Cl1'-Pb1-Cl1'''	84.95(1)	84.70(1)
Cl1''-Pb1-Cl2	90.00(1)	90.00(1)
Cl1'''-Pb1-Cl2	90.00(1)	90.00(1)
Cl1'''-Pb1-Cl2''	90.00(1)	90.00(1)
Cl1''-Pb1-Cl2''	90.00(1)	90.00(1)
σ(°)	3.0453	3.1960

i = 1-x,-y,z; ii = 1-x,y,-z; iii = x,-y,-z

Table S9. Bond angle variance of the individual $PbCl_6$ octahedra in phase **II** at different temperature.

Bond Angles (°)	360 K	340 K
Cl1-Pb1-Cl2	89.91(1)	90.02(1)
Cl1-Pb1-Cl1'	95.02(1)	95.81(1)
Cl1-Pb1-Cl1'''	84.66(1)	84.17(1)
Cl1-Pb1-Cl2'	89.91(1)	90.02(1)
Cl1''-Pb1-Cl2	90.09(1)	89.99(1)
Cl1''-Pb1-Cl1'	84.66(1)	84.17(1)
Cl1''-Pb1-Cl2'	90.09(1)	89.99(1)
Cl1''-Pb1-Cl1'''	95.66(1)	95.85(1)
Cl1'-Pb1-Cl2	89.91(1)	90.02(1)
Cl1'''-Pb1-Cl2	90.09(1)	89.99(1)
Cl1'''-Pb1-Cl2'	90.09(1)	89.99(1)
Cl1'-Pb1-Cl2'	89.91(1)	90.02(1)
σ(°)	3.2239	3.5157

i = 1-x,y,0.5-z; ii = -0.5+x,-0.5+y,z; iii = 1.5-x,-0.5+y,0.5-z;

Table S10. Bond angle variance of the individual $PbCl_6$ octahedra in phase **III** at different temperature

Bond Angles (°)	320 K	300 K	280 K
Cl1-Pb1-Cl2	102.32(1)	103.30(1)	104.12(1)
Cl1-Pb1-Cl3	90.74(1)	90.87(1)	91.06(1)
Cl1-Pb1-Cl1''	83.80(1)	83.38(1)	83.13(1)
Cl1-Pb1-Cl3'	90.74(1)	90.87(1)	91.06(1)
Cl2''-Pb1-Cl2	84.97(1)	84.90(1)	84.98(1)
Cl2''-Pb1-Cl3	89.23(1)	89.11(1)	88.92(1)
Cl2''-Pb1-Cl3'	89.23(1)	89.11(1)	88.92(1)
Cl2''-Pb1-Cl1	88.91(1)	88.42(1)	87.77(1)
Cl2-Pb1-Cl3	90.13(1)	90.01(1)	89.95(1)
Cl3'-Pb1-Cl2	90.13(1)	90.01(1)	89.95(1)
Cl1''-Pb1-Cl3'	89.78(1)	89.88(1)	89.91(1)
Cl1''-Pb1-Cl3	89.78(1)	89.88(1)	89.91(1)
σ(°)	4.4632	4.7896	5.0574

i = x,0.5-y,z; ii = -0.5+x,0.5-y,0.5-z

Table S11. Bond angle variance of the individual $PbCl_6$ octahedra in phase **IV** at different temperature.

Bond Angles (°)	250 K	220 K	200 K	180 K	150 K	130 K	100 K
Cl1''-Pb1-Cl2	104.80(6)	105.73(6)	106.31(6)	106.98(8)	107.91(9)	108.47(9)	109.21(9)
Cl1''-Pb1-Cl3	91.02(6)	91.08(6)	91.09(6)	91.18(8)	91.15(9)	91.22(9)	91.6(1)
Cl1''-Pb1-Cl1	82.89(5)	82.51(5)	82.23(6)	81.93(8)	81.45(9)	81.19(9)	80.84(9)
Cl1''-Pb1-Cl4	91.15(6)	91.32(6)	91.33(6)	91.35(8)	91.44(9)	91.46(9)	91.6(1)
Cl2''-Pb1-Cl1	87.17(6)	86.54(6)	86.18(6)	85.81(8)	85.35(9)	85.07(9)	84.60(9)
Cl2''-Pb1-Cl2	85.14(6)	85.22(6)	85.29(7)	85.28(8)	85.29(9)	85.28(9)	85.35(9)
Cl2''-Pb1-Cl3	89.04(6)	88.87(7)	88.97(7)	88.86(9)	88.9(1)	88.9(1)	89.0(1)
Cl2''-Pb1-Cl4	88.84(6)	88.85(7)	88.80(7)	88.86(9)	88.9(1)	88.8(1)	88.8(1)
Cl1-Pb1-Cl3	90.13(6)	90.26(6)	90.49(6)	90.56(9)	90.87(9)	91.00(9)	91.17(9)
Cl1-Pb1-Cl4	90.19(6)	90.45(6)	90.53(6)	90.70(9)	90.81(9)	90.95(9)	91.15(9)
Cl2-Pb1-Cl3	89.63(6)	89.52(7)	89.30(7)	89.18(9)	88.84(9)	88.90(1)	88.6(9)
Cl2-Pb1-Cl4	89.76(6)	89.44(7)	89.35(7)	89.21(9)	89.12(9)	88.8(1)	88.8(1)
σ(°)	5.2751	5.5973	5.8009	6.0387	6.3684	6.5745	6.8427

i = x,0.5-y,0.5-z; ii = x,1.5-y,0.5+z

Table S12. The calculated (ω_{calc}) and scaled (ω_{SC}) wavenumbers together with PED for Tz^{+}.

ω_{calc} (cm^{-1})	PED (%)
3512	νNH(57)+νNH'(42)
3503	νNH'(57)+νNH(42)
3213	νCH'(84)+νCH(15)
3207	νCH(84)+νCH'(15)
1552	νNC(33)+νNC"(20)+ δHNN(17)+δHNC(15)
1507	νNC'(34)+ δHCN(19)+νNC"(12)
1400	δHNC(30)+ νNC"(14)+νNC(12)+δCNN(12)
1391	νNC(33)+δHNN(31)+δHCN(10)
1255	δHCN'(47)+νNC'(20)+δHNN(15)
1166	νNC"(23)+νNC'(17)+νNN(12)+δHNC(13)+δHCN'(18)
1152	δHCN(37)+νNC'(14)+νNC"(12)+νNN(12)
1083	νNN(40)+δHNC(24)+δNCN(11)
1039	δNNC(26)+ δHCN(22)+νNN(18)+δCNN(17)
948	δNCN(58)+νNN(14)
927	δCNN(45)+δNNC(35)
848	τHCNN'(64)+τHCNN(24)
827	τHCNN(56)+τHCNN'(28)
733	τHNNC(74)+τHNCN(18)
691	τHNCN(77)+τHNNC(20)
649	τCNNC(70)+τNCNN(19)
610	τNCNN(67)+τCNNC(19)+τHCNN(12)

Response to the comments of the crystallographic reviewer:

There are 14 Structures in this paper. We examined this file: 2314654-2314667

This is a multi-temperature series of the same material.

The space group is reported to be

P21/c 100-250 K

Pnma 280-320 K

Cmcm 340-360 K

Fmmm 370-390 K

triag2pbcl4_iv_100_00 (CCDC 2314654)

The residuals are very large in this structure. Max|min = 1.9|-5.7. The R factors are high, and GooF is also higher than expected.

All ADPs are strongly elongated, mostly along the a-axis. Something isn't right here.

The structure is refined as a twin, but BASF refines to 9.7 -- which is meaningless and I really don't understand why it is here. It also makes no difference for the refinement.

Platon ADDSYMM thinks that these structures should be in Pnma. How precisely has the beta angle been measured? *Could* this be 90 Degrees? It is by no means clear; a refinement in Pnma is slightly better than it is in P21/c, but still suffers from problems with elongated ADPs and large residuals.

When refining the structure with 'whole molecule' disorder, then much lower R factors will result (ok, there are more parameters, but still -- I am getting around 4.5%!).

The strange thing is that these issues are also present in all other P21/c structures -- but to a less and less extent.

There are a couple of other serious issue: It is not clear from the crystals size whether this was the same crystal or not, since the size is variously reported as 0.555 x 0.179 x 0.122 or as 0.56 x 0.18 x 0.12.

In any case, this crystal is **very much** to large to be suitable for this kind of experiment. The absorption coefficient μ is 13.7mm^-1 -- so the largest size is definitely not supposed to be any bigger than 1/14 mm. This unsuitably large crystal may contribute to the observed high variation in the Fobs vs Fcalc plot.

Although there are fewer problems with the higher-T structures, these could also benefit from re-measuring data on a more suitably-sized crystal. This is all the more the case since there are also space-group ambivalences here.

In the MS, bond distances and angles are quoted without e.s.d values; please provide these values.

In the MS, please provide at least one structural drawing showing ADPs of each structure. From these images, any disorder should be visible -- and the nature of the actual molecule must be easily discernible.

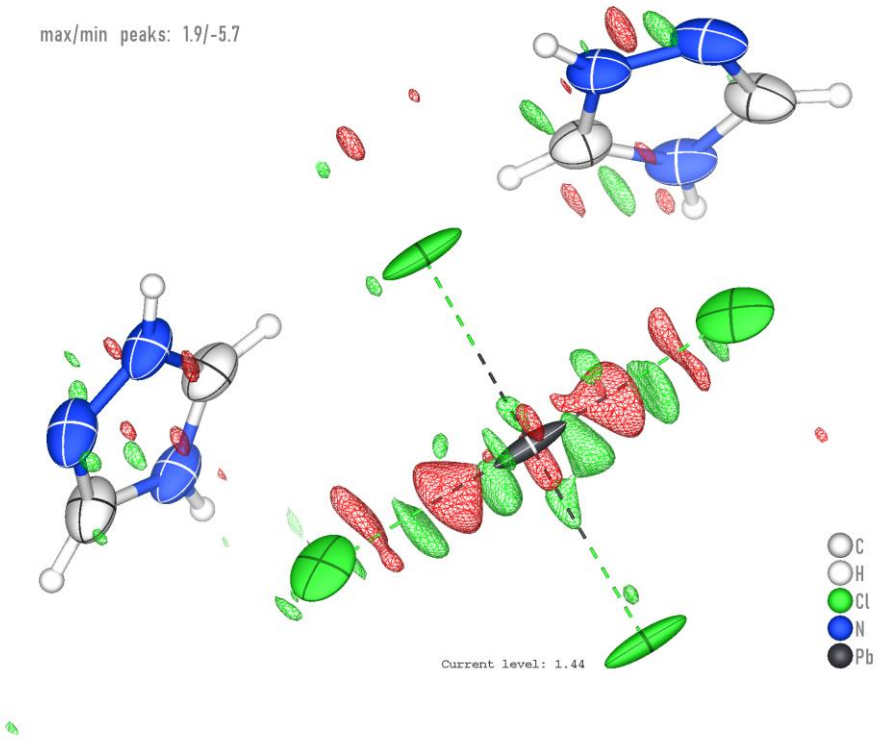
In summary, I do not think that these structures provide any detailed information about phase changes at all: there is ambivalence in almost all structures with respect to the space groups. New structures, based on crystal of suitable size, might.

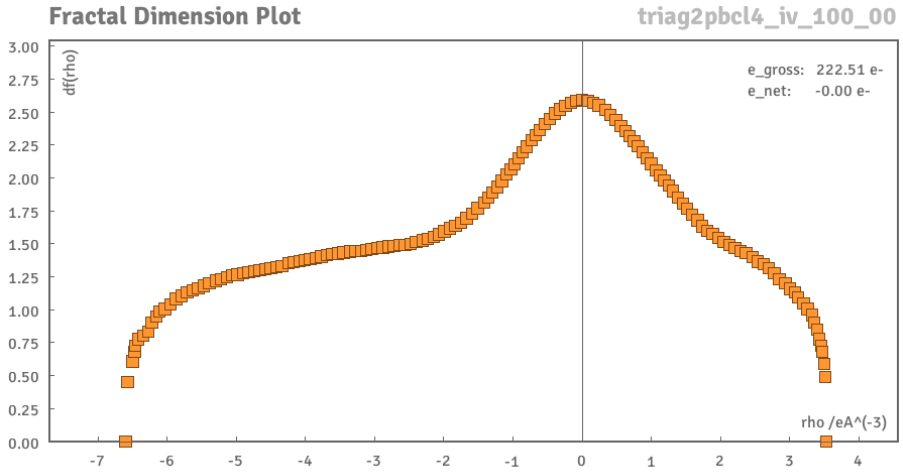
Author response:

Thank you for your thorough review of our crystallographic data and for the insightful comments. We appreciate the opportunity to address the concerns you have raised.

1. **Structure and Space Group Assignment**: *We acknowledge your observation regarding the assignment of space groups across different temperature ranges. The choice of monoclinic symmetry was a pivotal aspect of our study. This assignment was based on Differential Scanning Calorimetry (DSC) measurements, supported by Raman and Second Harmonic Generation (SGH) measurements and the details regarding the space group selection for phase IV was described in Discussion chapter of our article. In all our structural experiments, the beta angle was measured to three decimal places with esd not exceeding 0.006°. To further clarify this important issue, we have added the plot of the monoclinic strain as a function of temperature. The strain is weak, which explains the result of the PLATON report.*

2. **Residual density and ADPs**: *We understand your concerns about the large residuals and elongated ADPs, predominantly along the a-axis, as shown in the figures below (similar images and graphs could be obtained for $P2_1/c$ at other temperatures). These observations were intriguing to us as well and led to a deeper investigation into the underlying crystallography. The refinement as a twin and the inclusion of BASF was an attempt to account for the observed anomalies, albeit not providing a significant improvement in the refinement quality. We repeated the refinement without TWIN and resubmitted the CIFs. The residual density peaks indeed occur in our crystallographic data (see the figures below for the structure at 100K; similar images and graphs could be obtained for all $P2_1/c$ structures reported in this paper) however they are consistently located around the central Pb^{2+} cations, which is typical for very heavy atoms.*





3. **Crystal Size and Suitability**: *We agree with your observation regarding the crystal size being larger than ideal for X-ray diffraction experiments. It's a valid point that large crystals can lead to high variation in the Fobs vs Fcalc plot due to absorption issues. However, we encountered a challenge with our crystals growing large, and our experience suggests that cutting them could introduce defects that significantly hamper structural determination, especially for phase IV, which shows strong pseudosymmetry toward the orthorhombic system. To overcome this challenge, we designed an*

experimental strategy employing a bisecting mode positioning of the sample to minimize absorption in the needle-like crystal aligned along the diffractometer phi axis. Indeed, this approach should had been explained in Experimental, which we have done in the revised manuscript. This approach was a compromise to balance crystal integrity and experimental feasibility.

4. **Reporting of Bond Distances and Angles**: *We acknowledge the omission of e.s.d values for bond distances and angles in the manuscript (MS) and will ensure these are included in the revised manuscript.*

5. **Structural Drawings and Disorder Visibility**: *We appreciate your suggestion to include structural drawings showing ADPs for each structure. This addition will indeed help in visualizing any disorder and making the nature of the molecule more discernible. We will incorporate these drawings in the revised supporting information*.

6. **ESD values:** Thank you for pointing out the lacking e.s.d values for bond distances and angles in our article. We acknowledge this oversight and have now included these values in the revised manuscript and SI to provide a more complete and accurate representation of our findings.

In summary, we recognize the validity of your concerns and are committed to addressing them thoroughly in our revised manuscript. We believe that with the proposed amendments, our study will provide more robust and clear insights into the phase changes and structural characteristics of the material under investigation. Thank you once again for your constructive feedback.

We also include checkCif alerts at the end of SI

Table S13. Raman and IR wavenumbers (in cm^{-1}) of Tz_2PbCl_4 at various temperatures together with the proposed assignment.[a]

RS 380 K	IR 370 K	RS 300 K	IR 300 K	RS 80 K	IR 10 K	Pol. RS	Calc.	assignment
3230sh	3236m,vb	3213sh	3228m,vb	3210sh	3218m		3512	νN-H ip
		3130w		3140w+3130w				overtone/combination
3097vw		3096w		3106w+3092w				overtone/combination
	3072s		3075s		3097s+3081s		3503	νN-H icp
3155m	3166m	3153m	3167m	3154m	3173m	3149m	3213	νC-H ip
	3120m		3121m		3121m		3207	νC-H icp
3037w	3034w	3036w	3036w	3007w+2987w		3040w		overtone/combination
2936w	2924m	2935w+ 2915sh	2923w	2933w+2924w + 2909w	2921w	2936w		overtone/combination
	2900m		2900w		2896w			overtone/combination
2811w	2795w	2815w	2796w	2820w	2794vw	2816w		overtone/combination
1561vw	1556s	1561vw	1554s	1562vw	1551s	1562w	1552	νC-N, δN-H
1533vw	1527s	1534vw	1527s		1529s+1521s	1533m	1507	νC-N. δC-H
1417vw	1406m	1419w	1407m	1423w	1410w+1404m	1421w	1400	δN-H, νC-N
1393vw	1390m	1392w	1389s	1388w	1395w+1384s	1392s	1391	νC-N, δN-H
1317vw		1318vw		1319vw		1318w		overtone/combination
1263s	1255w	1261s	1253w	1257s+1250m	1250w+1248w	1262s	1255	δC-H
	1236w		1237w		1240w+1235w	1240vw		overtone/combination

	1175w		1174w		1173w			overtone/combination
1175s	1163s	1173s	1162s	1170s	1157s	1173s	1166	νC-N, δC-H
1156w	1147m	1154m	1147s	1153m	1145w	1155m	1152	δC-H, νC-N
1112w	1100w	1111w	1099w	1110vw	1101w+1095w	1112s	1083	νN-N
1037m	1033s	1037m	1032s	1038m	1032s	1038m	1039	δNNC, δC-H
	952sh		954w		953w			overtone/combination
956m	947s	955m	947s	955s	947s	955s	948	δNCN
942vw	939sh	941w	939sh	940w	938w	942w	927	δCNN, δNNC
			889w		899w+894w	895w		overtone/combination
	866m		867m	856vw	868m+865sh		848	γC-H ip
					843w+835w			overtone/combination
	816sh		817sh	835w	822m+817m		827	γC-H icp
	782s,vb		783s,vb	791w	799s+789s		733	γN-H ip
	736sh		740m		741m+735sh		691	γN-H icp
	658s+655s		658s+655s		659s+655s	659w	649	γ_{ring} CNNC
	618s		619s		620s+618sh	623w	611	γ_{ring} CNCN
497w,b		493w,b		491w,b				T’
		201w		204w				L+ T’+ Pb-Cl stretch
174sh		176w		188w+180w				L+ T’+ Pb-Cl stretch
124m		127m		139m				L+ T’+ Pb-Cl stretch

	116m	135m	L+ T'+ Pb-Cl stretch
		120m+110w	L+ T'+ Pb-Cl stretch
	80m	86w+80w	L+ T'+ Pb-Clstretch
		73w+70w	Pb-Cl bend
56s	60s	66m+62s	Pb-Cl bend
34s	49m	50s	Pb-Cl bend
20s	26vs	32s	L($PbCl_6$)

[a] key: vs, very strong; s, strong; m, medium; w, weak; vw, very weak; sh, shoulder; b, broad; vb, very broad; ν, stretching; δ, in-plane bending; γ, out-of-plane bending; ip, in-phase; icp, in-counterphase; L, librational mode of organic cation; T', translational mode of organic cation.

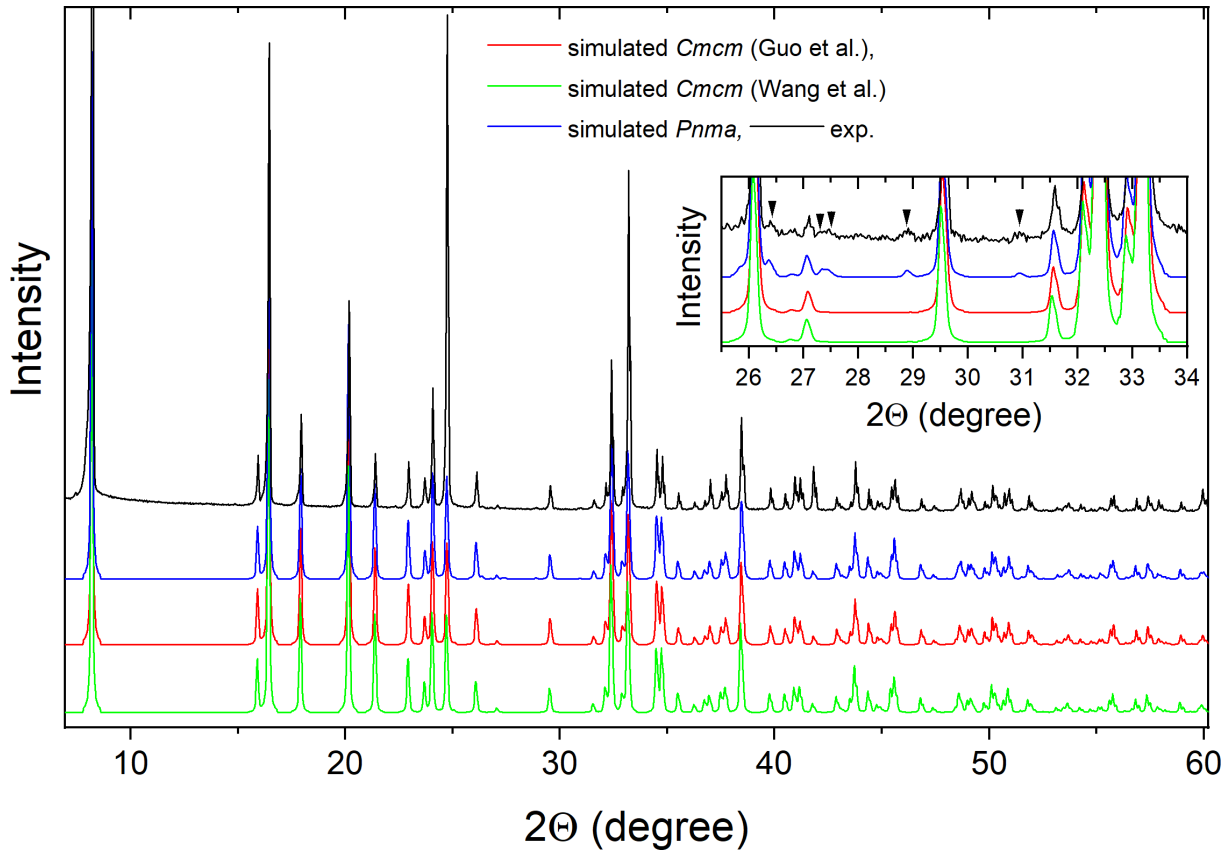


Fig. S1. Powder XRD pattern for Tz_2PbCl_4 together with the calculated one based on the *Pnma* (300 K, this work), *Cmcm* (298 K, Guo *et al.*)[1] and *Cmcm* (300 K, Wang *et al.*)[2] single crystal structure of Tz_2PbCl_4. Inset shows details for weak reflections in the 25.5-34° range. Arrows indicate reflections which are consistent with the *Pnma* symmetry but do not appear in the simulated patterns based on the *Cmcm* symmetry.

References

1. Y. Y. Guo, L. J. Yang, J. A. McNulty, A. M. Z. Slavin and P. Lightfoot, Structural Variations in (001)-oriented Layered Lead Halide Perovskites, Templated by 1,2,4-Triazolium, *Dalton Trans.*, 2020, **49**, 17274−17280.

2. Z. Wang, X. Chen, Y. Song, Z. Du, Y. Zhou, M. Li, W. Huang, Q. Xu, Y. Li, S. Zhao and J. Luo, A Two-Dimensional Hybrid Perovskite with Heat Switching Birefringences, *Angew. Chem. Int. Ed.*, 2023, **62**, e202311086.

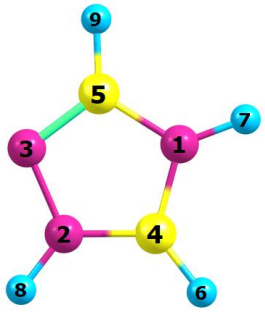


Fig. S2. Numbering of atoms in 1,2,4-triazol cation.

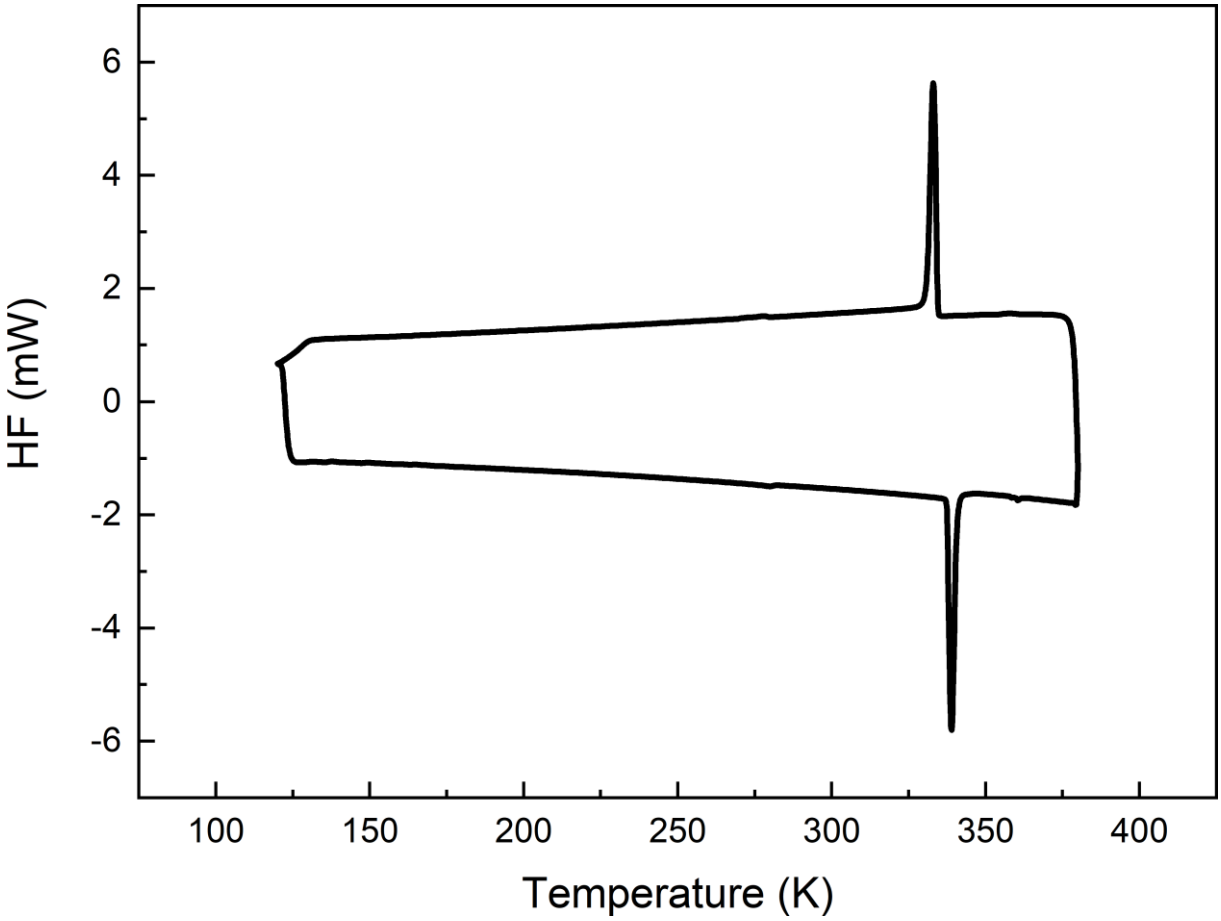


Fig. S3. DSC thermogram for Tz_2PbCl_4 in heating and cooling mode.

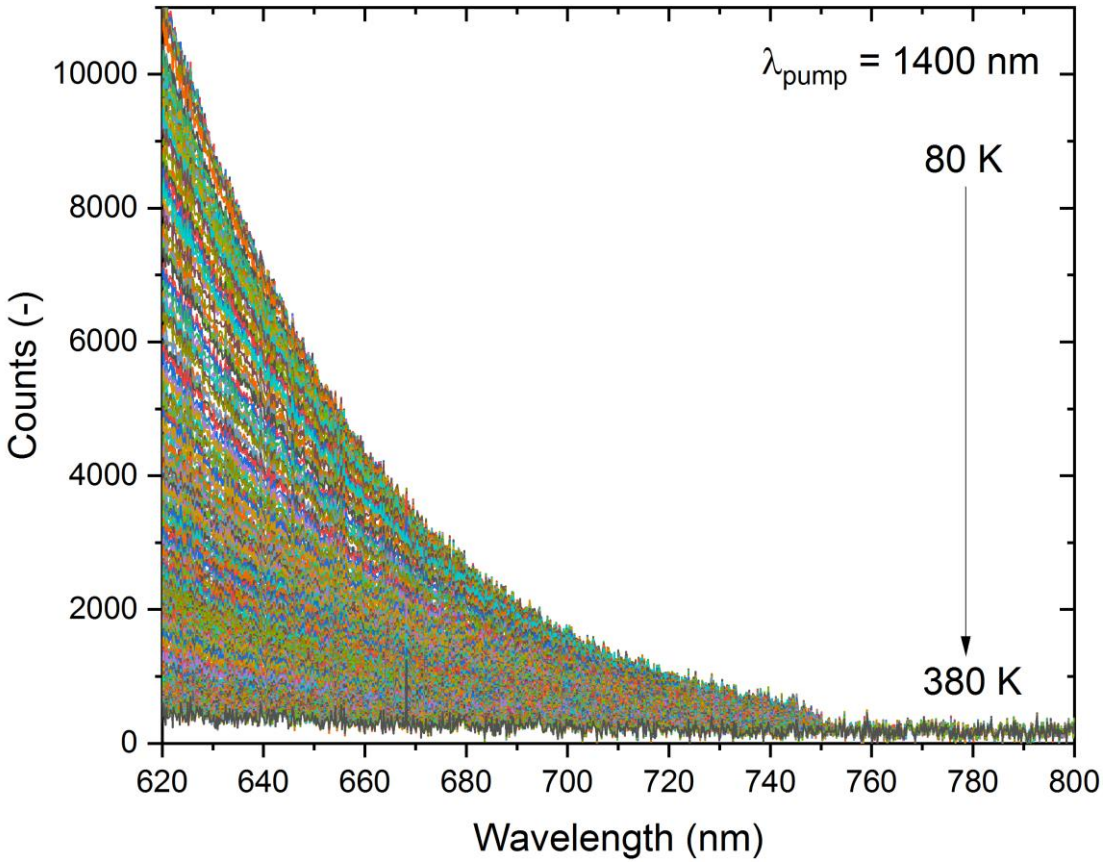


Fig. S4. Overlay of experimental spectra obtained upon irradiation of Tz_2PbCl_4 with 1400 nm femtosecond laser pulses during heating run from 80K to 380K. The only nonlinear optical emission present in this spectrum is the long-wavelength tail of the multi-photon excited luminescence. The shoulder at around 750 nm is due to the short-pass optical filter centered at that wavelength. Note the lack of SHG response at λ/2 (700 nm) confirms the structural centrosymmetry of Tz_2PbCl_4 across all crystal phases.

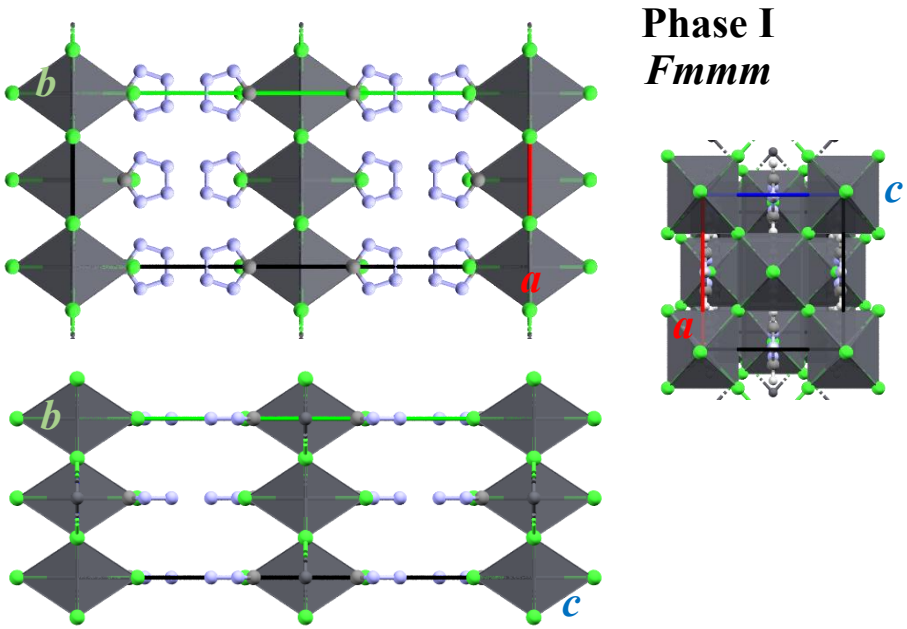


Fig. S5. Crystal structure of Tz_2PbCl_4 phase I projected along all crystal directions.

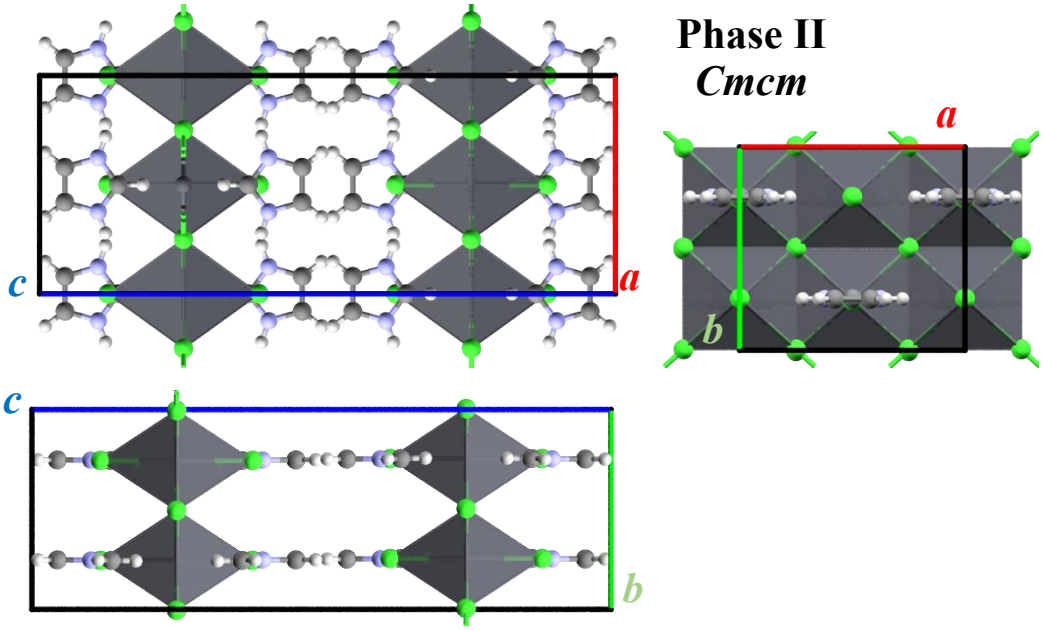


Fig. S6. Crystal structure of Tz_2PbCl_4 phase II projected along all crystal directions.

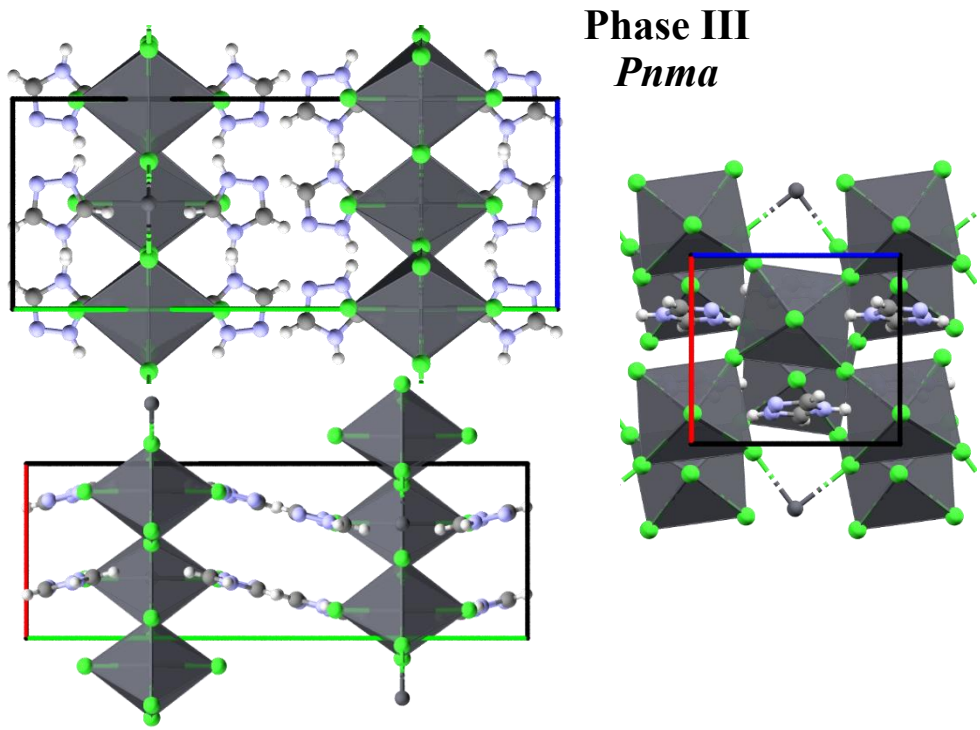


Fig. S7. Crystal structure of Tz_2PbCl_4 phase III projected along all crystal directions.

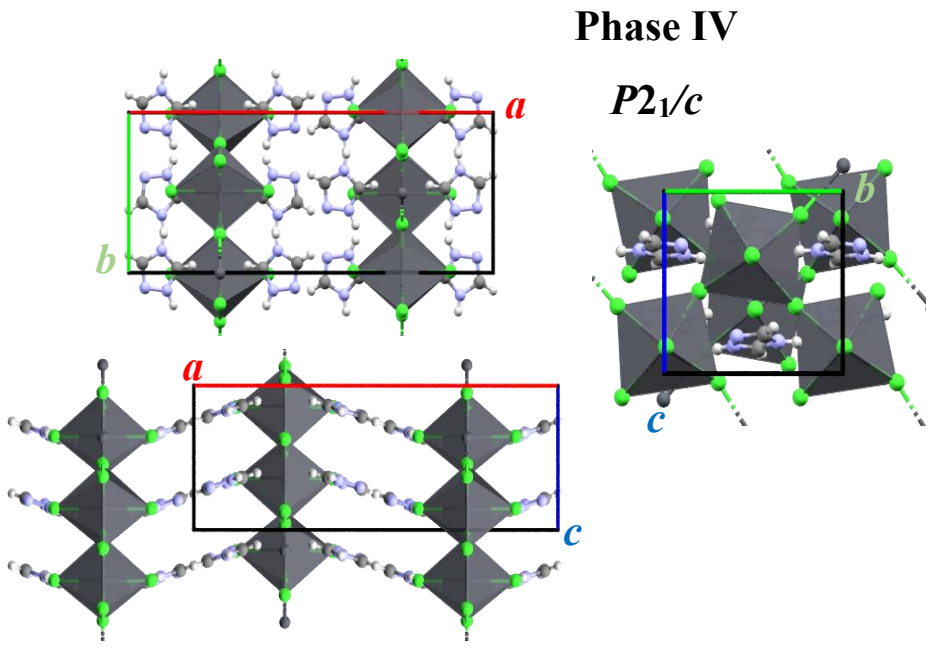


Fig. S8. Crystal structure of Tz_2PbCl_4 phase IV projected along all crystal directions.

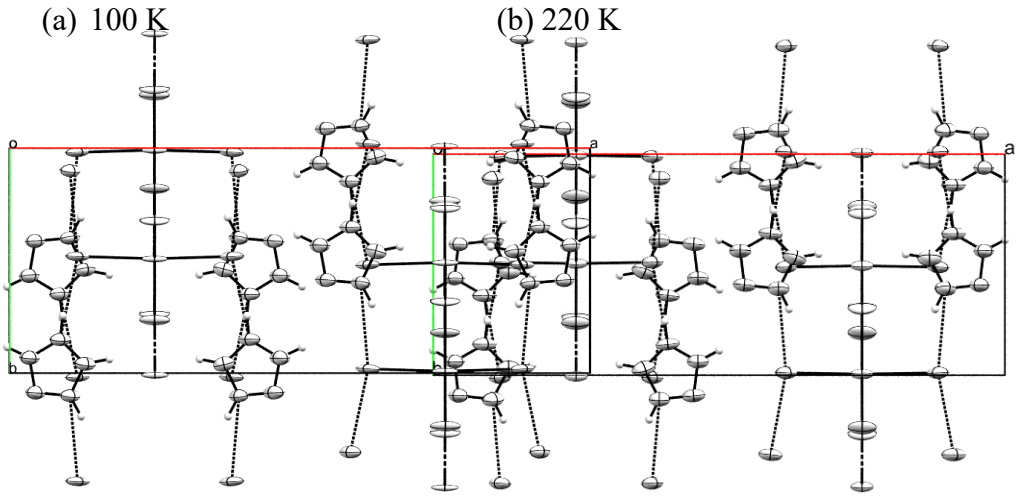


Fig. S9. The ORTEP diagram of Tz_2PbCl_4 phase IV at (a) 100 K and (b) 220 K. Thermal ellipsoids are at 50% probability level. Dashed lines indicates the hydrogen bonds.

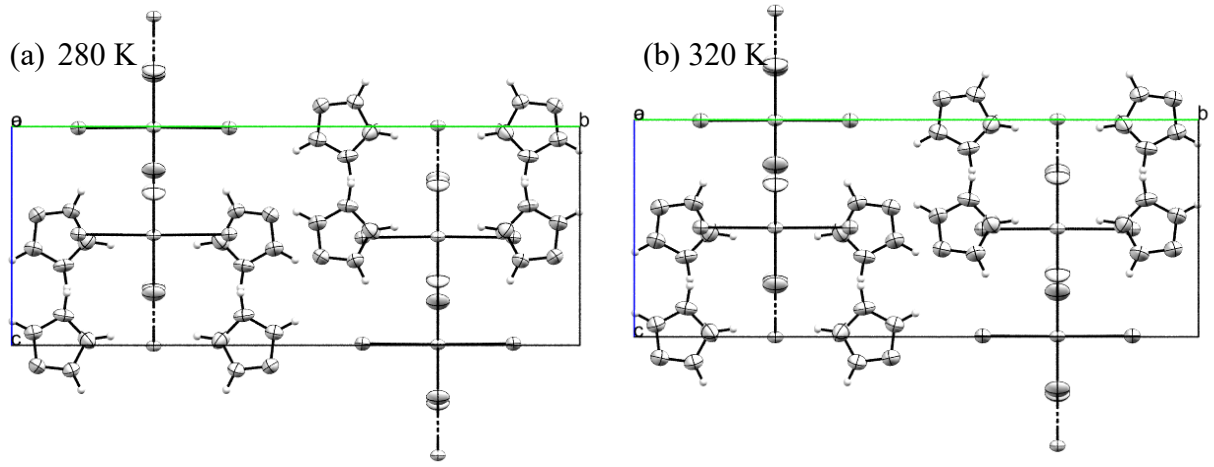


Fig. S10. The ORTEP diagram of Tz_2PbCl_4 phase III at (a) 280 K and (b) 320 K. Thermal ellipsoids are at 50% probability level. Dashed lines indicates the hydrogen bonds.

(a) Phase II at 340 K

(b) Phase I at 370 K

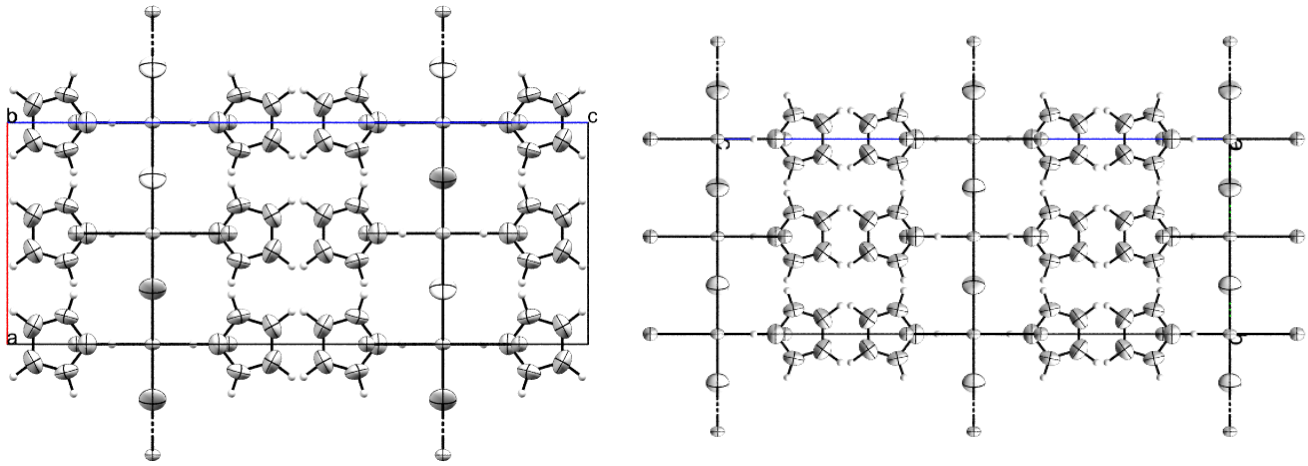


Fig. S11. The ORTEP diagram of Tz_2PbCl_4 in (a) phase II at 340 K and (b) in phase I at 370 K. Thermal ellipsoids are at 50% probability level. Dashed lines indicates the hydrogen bonds.

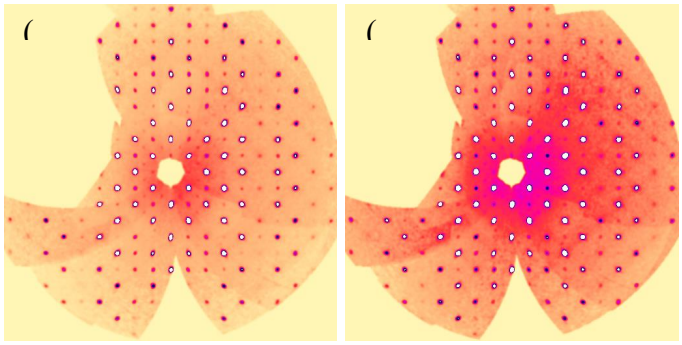


Fig. S12. The reconstructed *hk*0 layer reconstructed from the measurements collected (a) at 280 K and (b) 300 K showing the presence of odd *h* +*k* reflections.

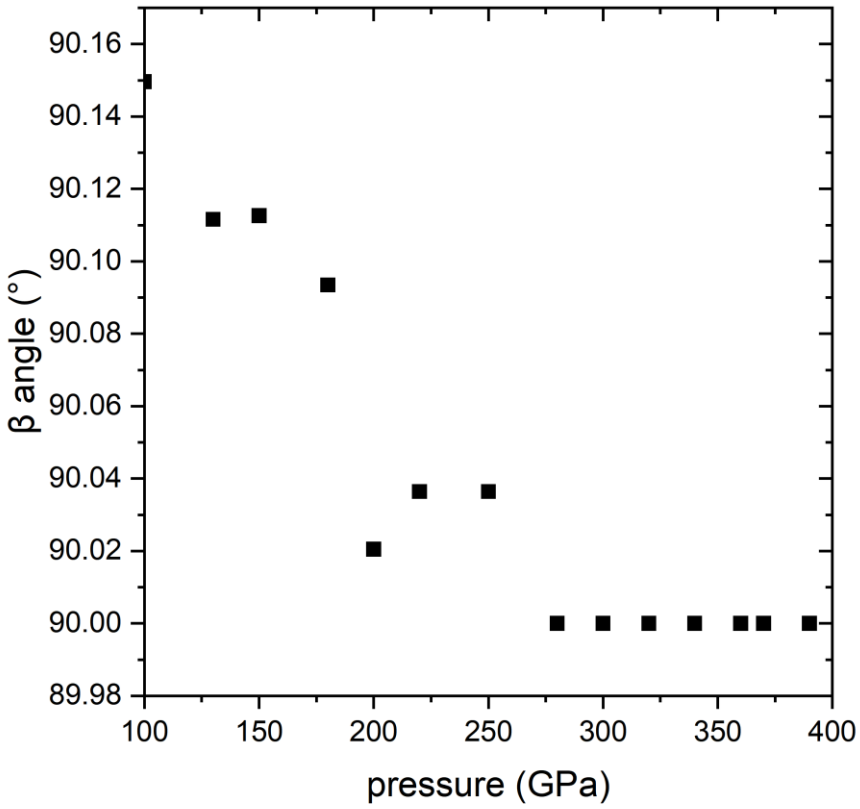


Fig. S13. The change of the β along plotted in the function of temperature. The ESD are smaller than symbols.

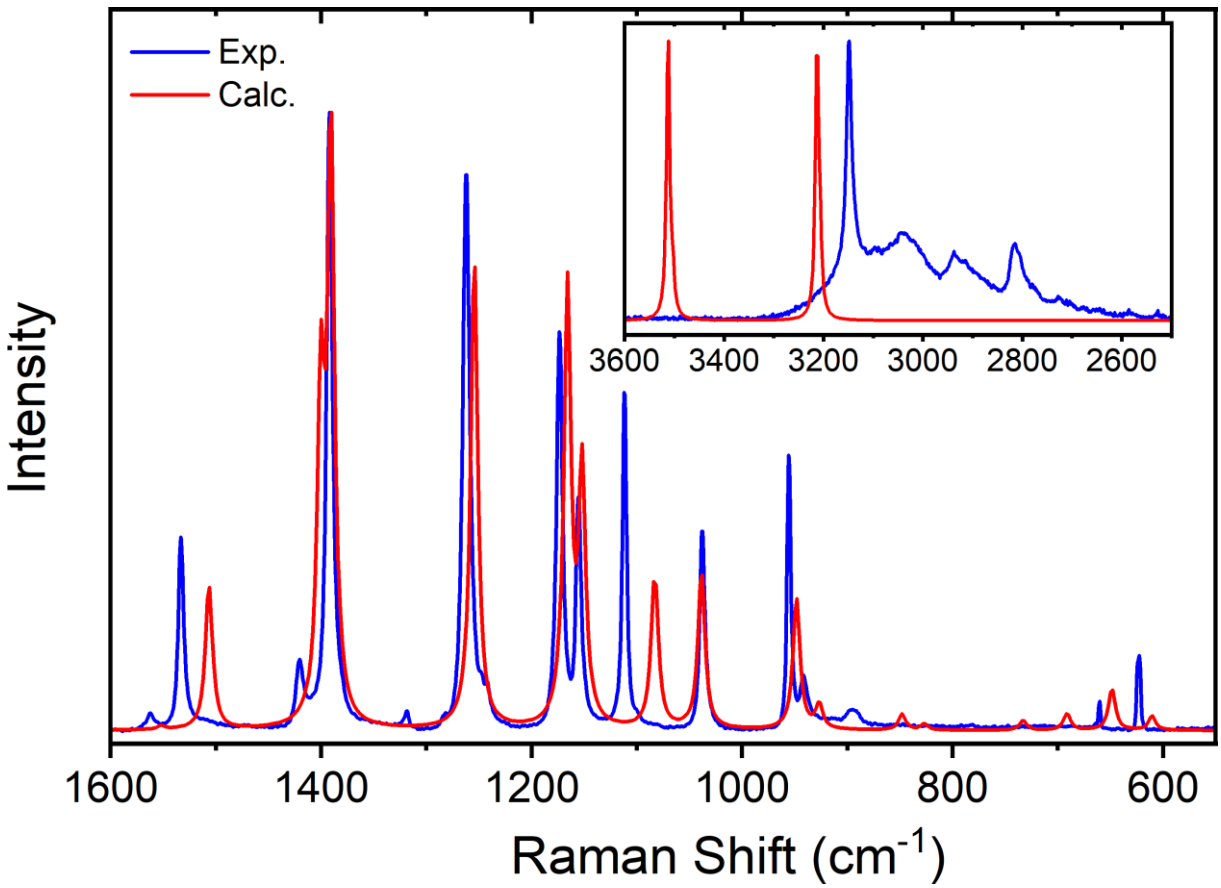


Fig. S14. Experimental Raman spectrum of polycrystalline Tz_2PbCl_4 (blue) and calculated Raman spectrum of 1,2,4-triazolium cation (red).

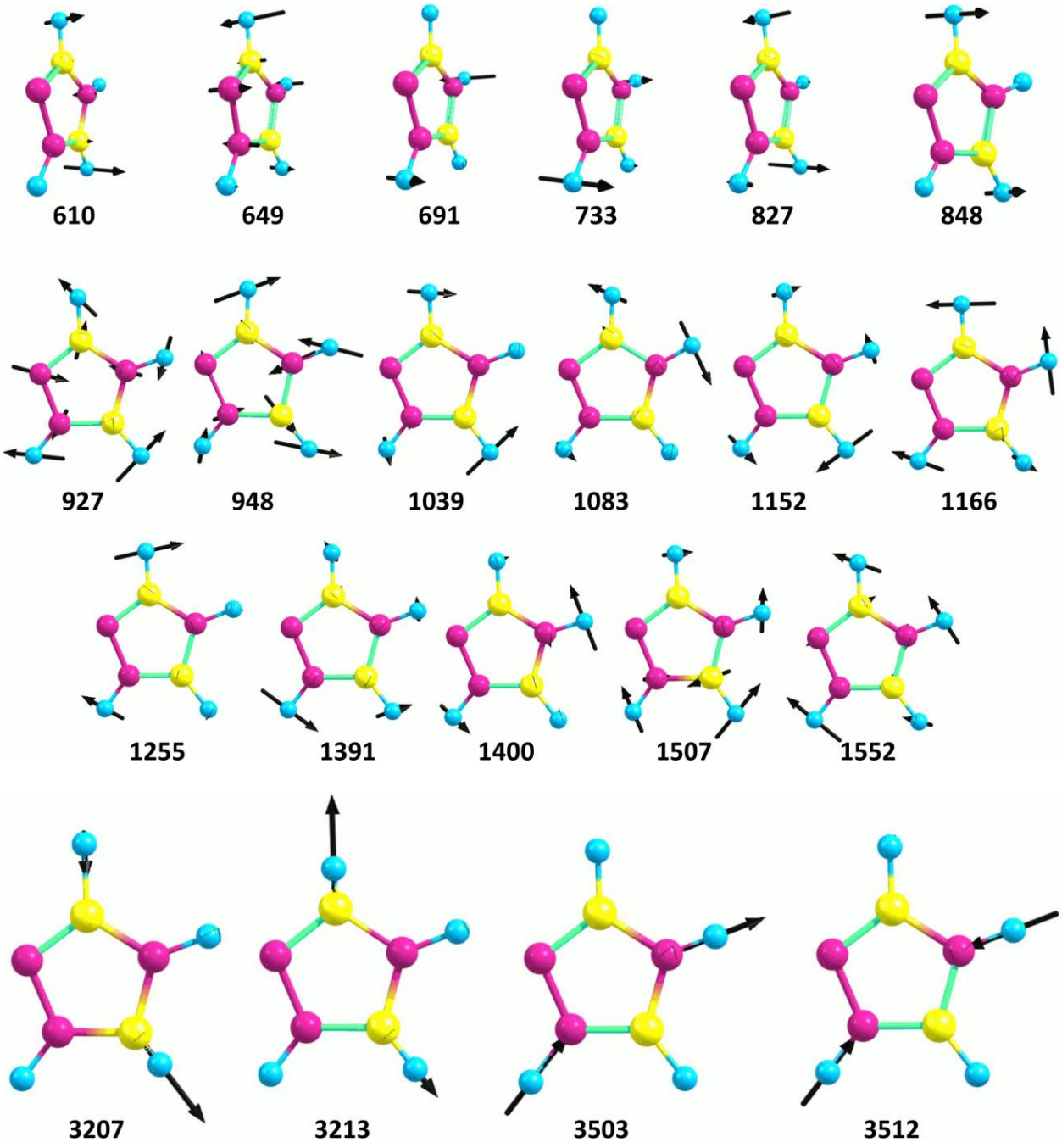


Fig. S15. Displacement of atoms for all calculated vibrational modes.

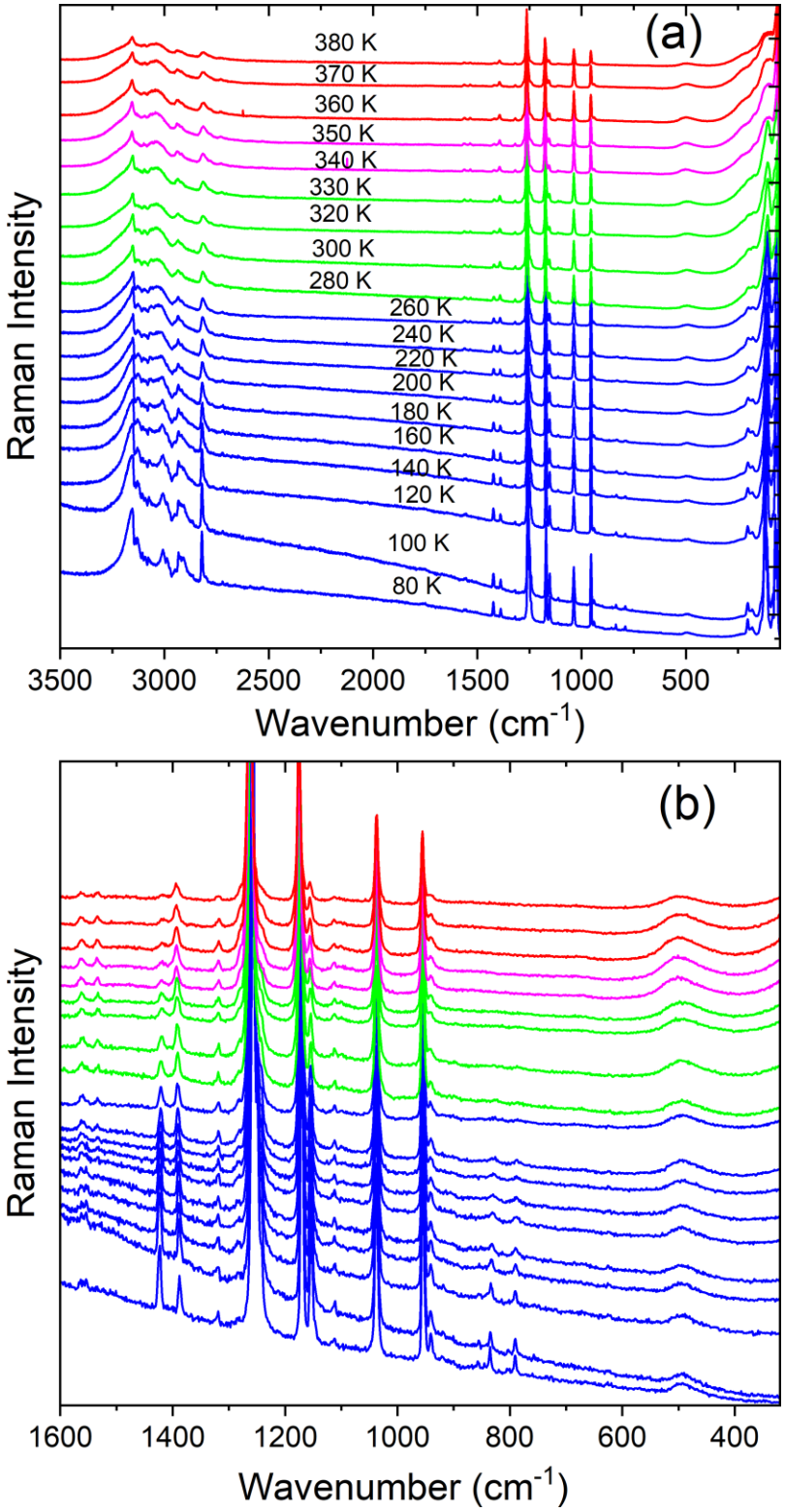

(a)
380 K
370 K
360 K
350 K
340 K
330 K
320 K
300 K
280 K
260 K
240 K
220 K
200 K
180 K
160 K
140 K
120 K
100 K
80 K
Raman Intensity
3500
3000
2500
2000
1500
1000
500
Wavenumber (cm-1)
(b)
Raman Intensity
1600
1400
1200
1000
800
600
400
Wavenumber (cm-1)

Fig. S16. (a) Temperature-dependent Raman spectra in the 3500-50 cm^{-1} and (b) enlarged1600-350 cm^{-1} range to show details for weaker Raman bands.

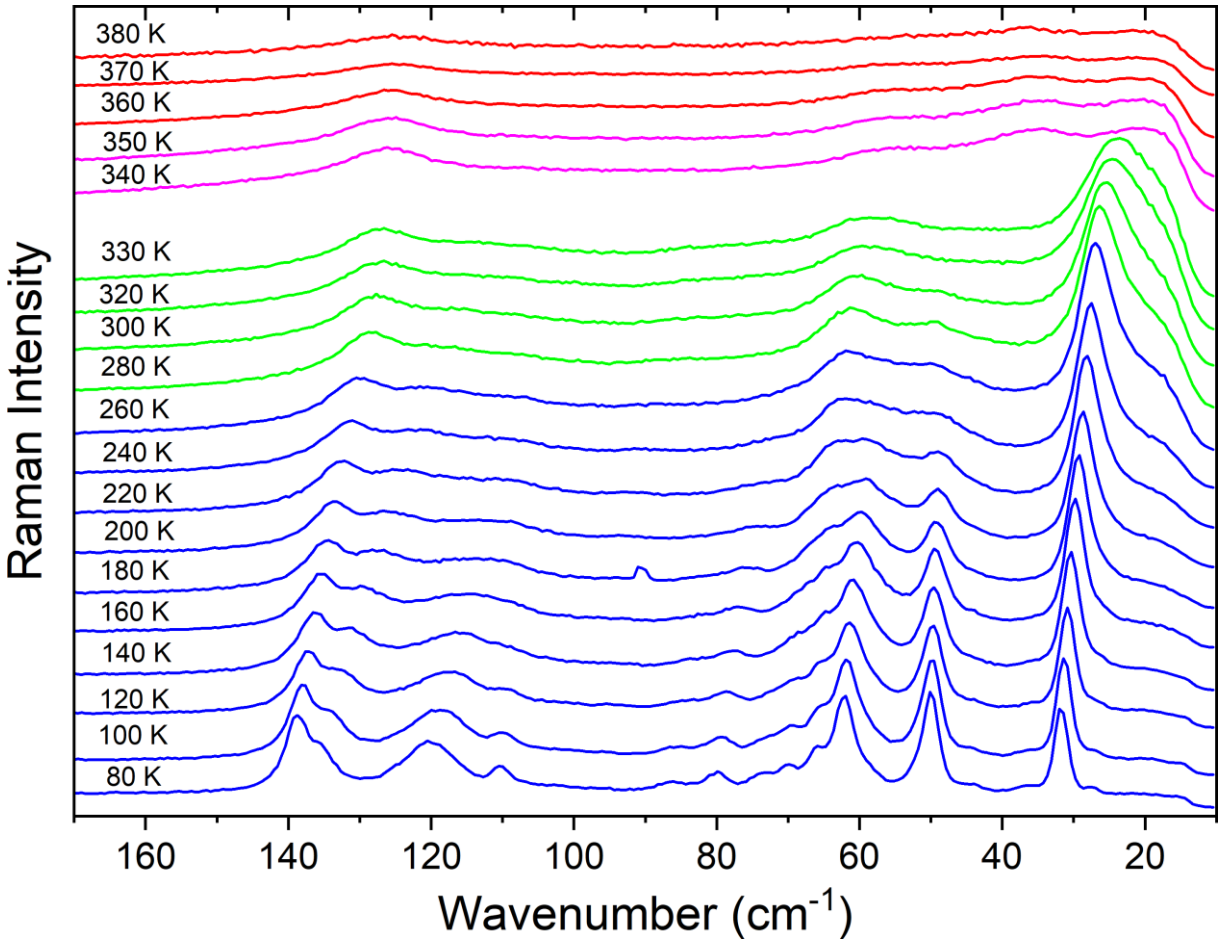


Fig. S17. Temperature-dependent Raman spectra in the 170-10 cm^{-1} range.

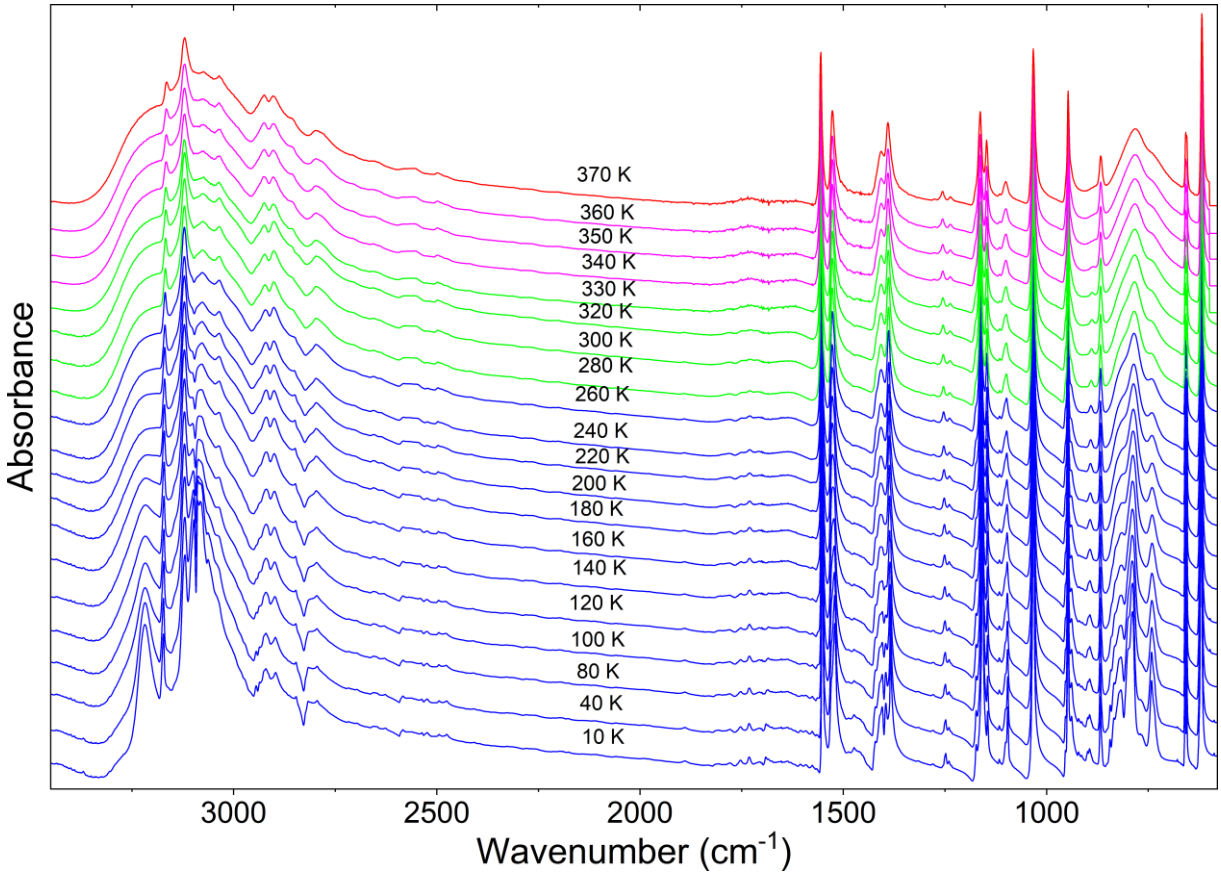


Fig. S18. Temperature-dependent IR spectra in the 3450-580 cm^{-1} range.

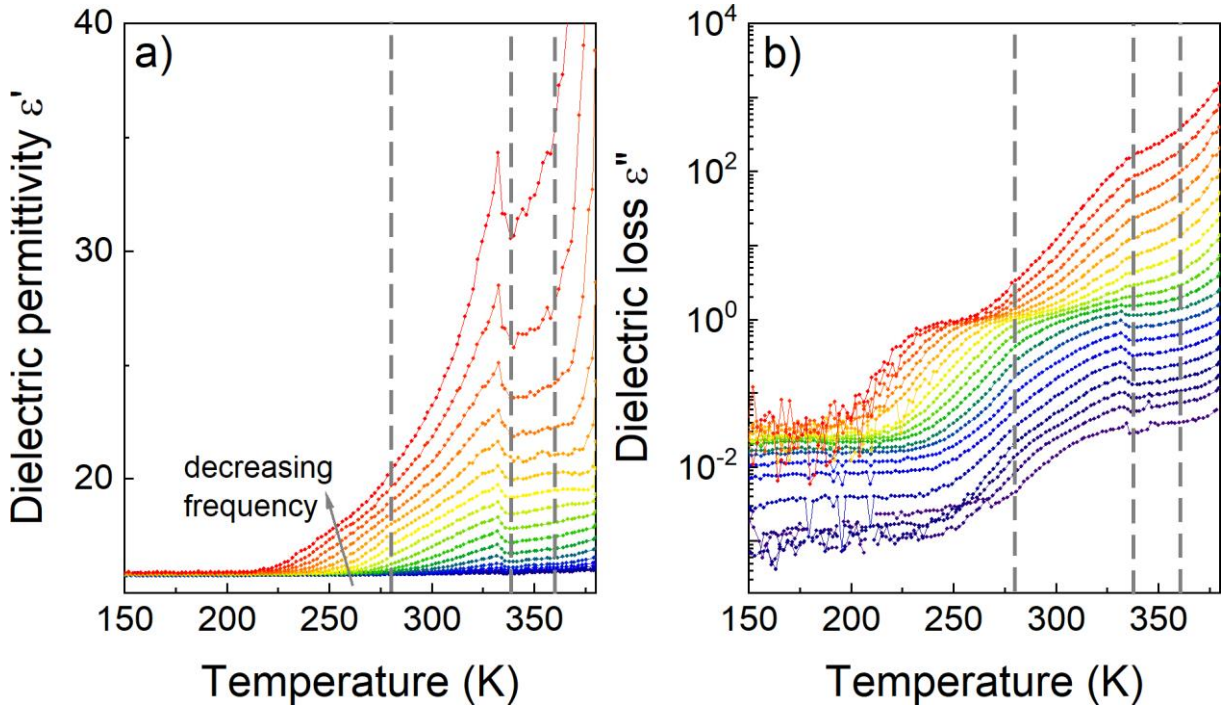


Fig. S19. Temperature dependence of (a) dielectric permittivity and (b) dielectric loss for selected frequencies. The vertical dashed lines indicate phase transition temperatures.

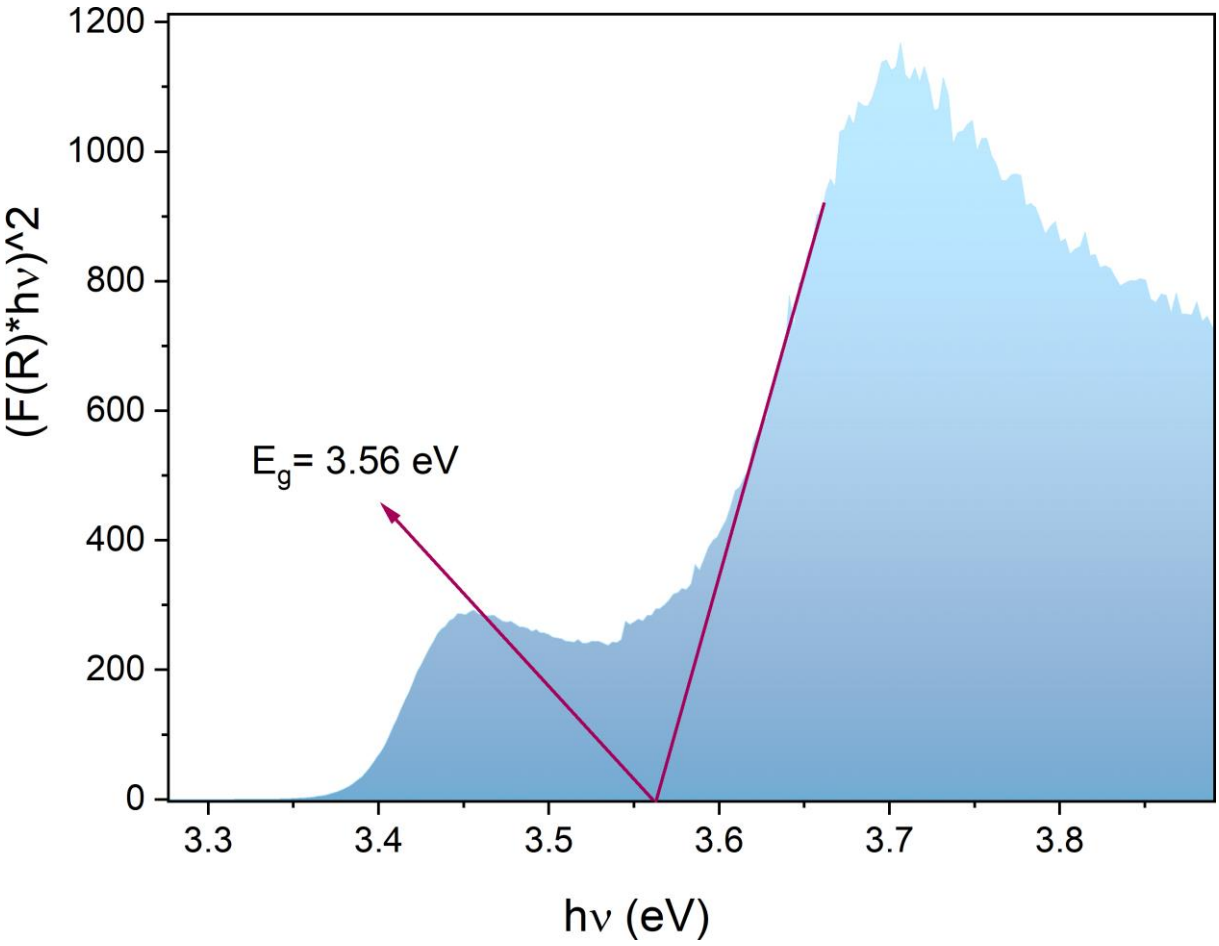


Fig. S20. Band gap (E_g) estimation with Tauc plot for Tz_2PbCl_4.

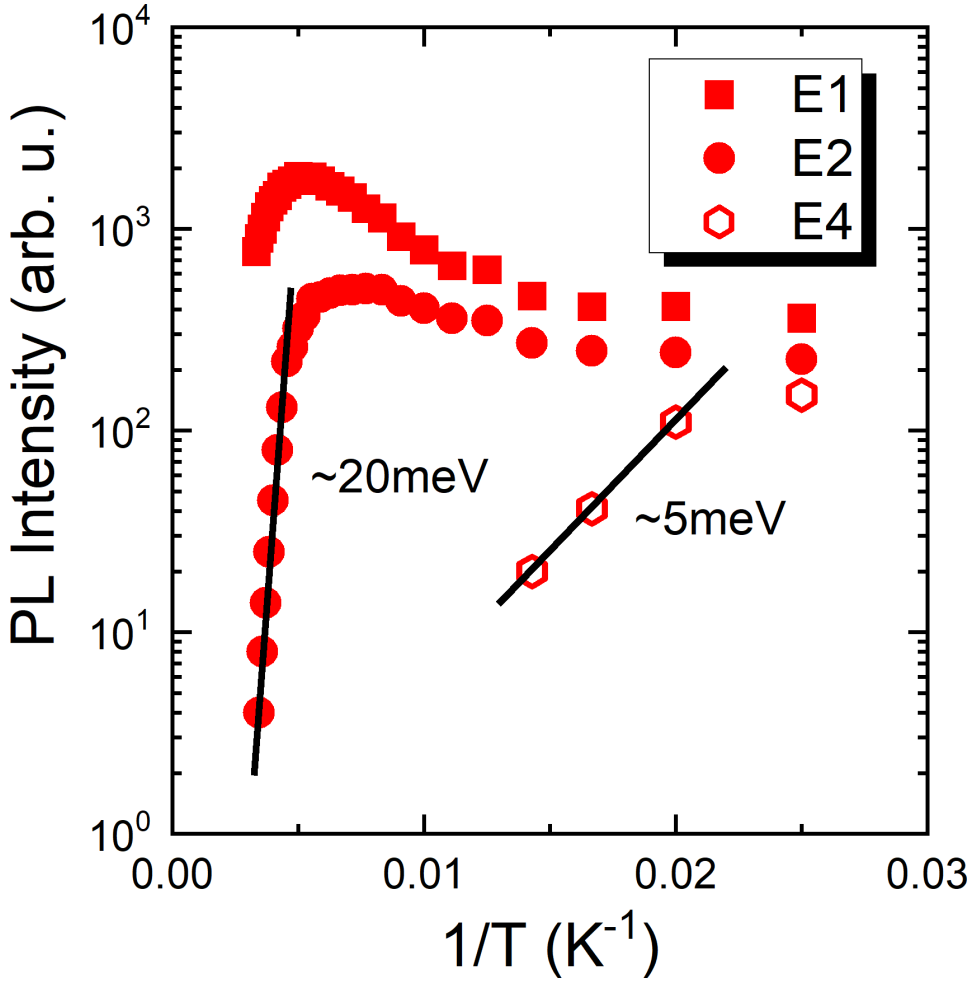


Fig. S21. Emission integrated intensity of E1, E2 and E3 plotted on a 1/T scale. Activation energies are determined according to the formula: $I(T) \propto exp(-E_a/kT)$, where I is the intensity, E_a is the activation energy and T is the temperature.

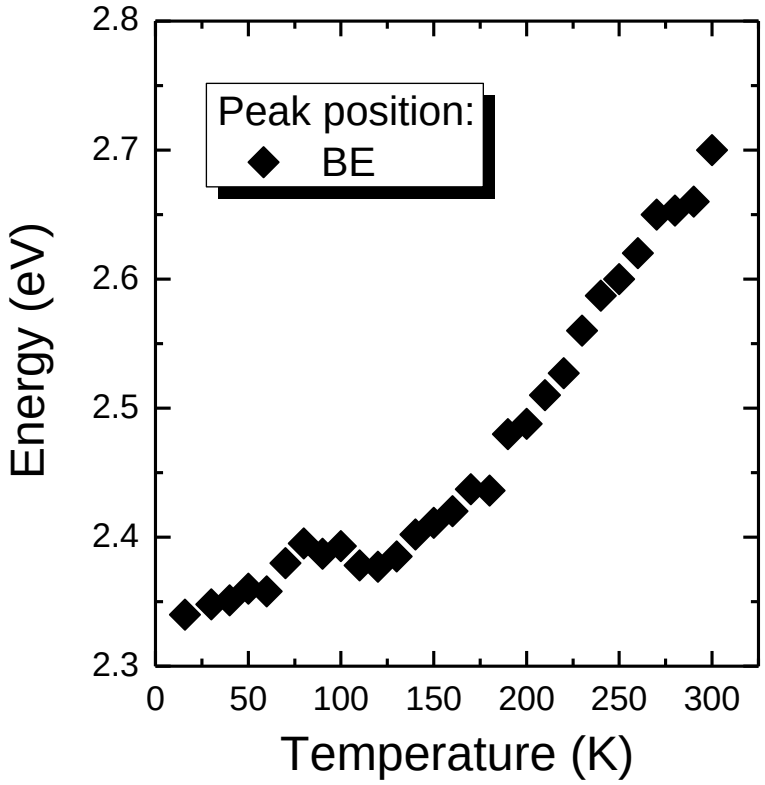


Fig. S22. Temperature dependence of the positions of BE PL peak.

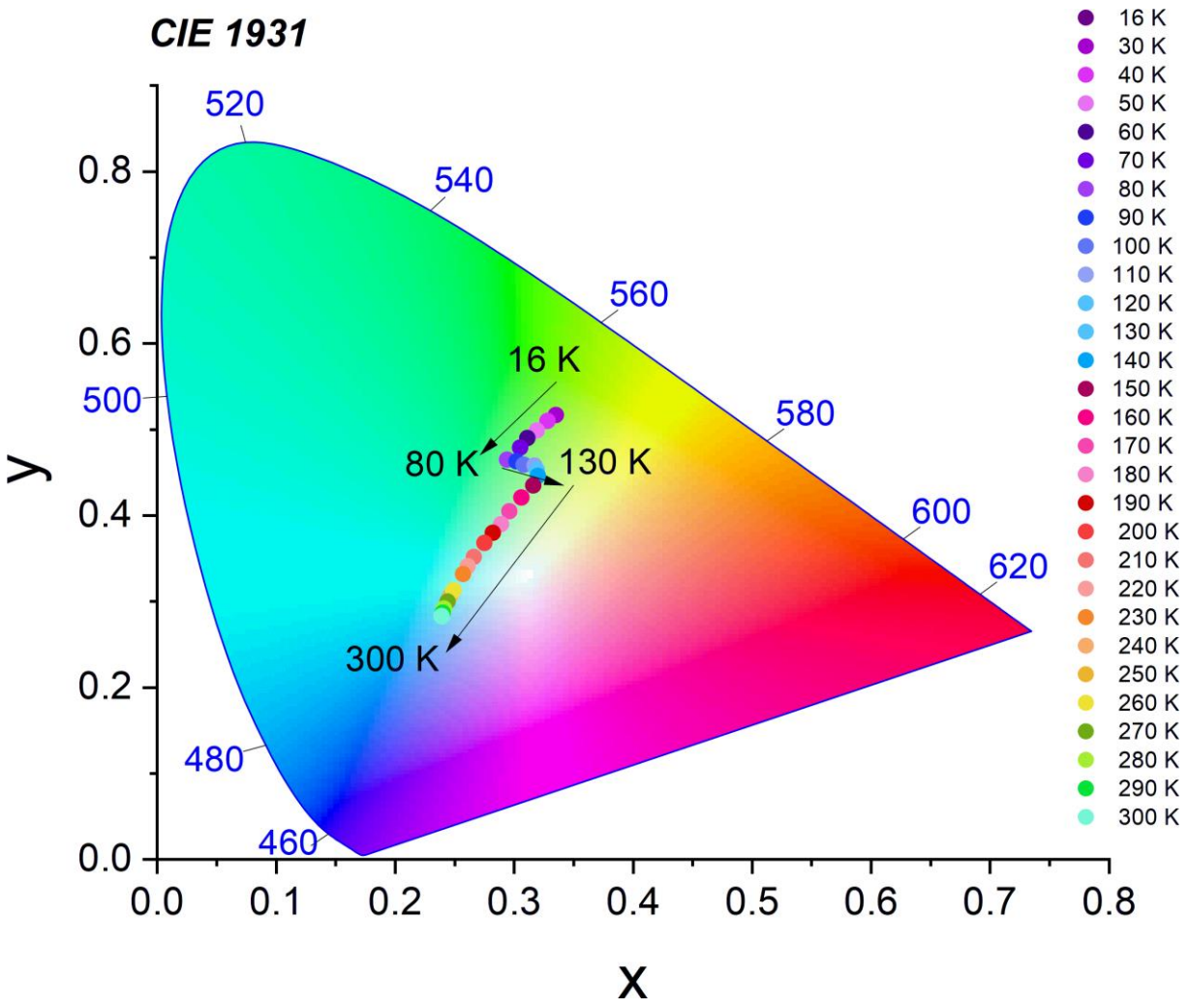


Fig. S23. CIE coordinates of Tz_2PbCl_4 crystal.

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) triag2pbcl4_i_370_00, triag2pbcl4_i_390_00, triag2pbcl4_ii_340_00, triag2pbcl4_ii_360_00, triag2pbcl4_iii_280_00, triag2pbcl4_iii_300_00, triag2pbcl4_iii_320_00, triag2pbcl4_iv_100_00, triag2pbcl4_iv_130_00, triag2pbcl4_iv_150_00, triag2pbcl4_iv_180_00, triag2pbcl4_iv_200_00, triag2pbcl4_iv_220_00, triag2pbcl4_iv_250_00

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: triag2pbcl4_i_390_00

Bond precision: N- C = 0.0110 A			Wavelength=0.71073
Cell:	a=7.6009(7)	b=8.3017(6)	c=21.798(2)
	alpha=90	beta=90	gamma=90
Temperature:	390 K		
	Calculated		Reported
Volume	1375.5(2)		1375.4(2)
Space group	F m m m		F m m m
Hall group	-F 2 2		-F 2 2
Moiety formula	4(Cl Pb0.25), 2(C2 H4 N3) Cl4 Pb, 4(C H2 N1.5)		
Sum formula	C4 H8 Cl4 N6 Pb		C4 H8 Cl4 N6 Pb
Mr	489.16		489.15
Dx,g cm-3	2.362		2.362
Z	4		4
Mu (mm-1)	13.022		13.023
F000	896.0		896.0
F000’	885.70		
h,k,lmax	10,11,29		10,11,29
Nref	539		513
Tmin,Tmax	0.110,0.210		0.069,1.000

Tmin’ 0.001

Correction method= # Reported T Limits: Tmin=0.069 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 0.952 Theta(max)= 29.013 wR2(reflections)=

R(reflections)= 0.0251(512)

0.0525(513)

S = 1.038 Npar= 30

The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level**. Click on the hyperlinks for more details of the test.

Alert level C

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.975 Why?

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check

Calc: 4(Cl Pb0.25), 2(C2 H4 N3)

Rep.: Cl4 Pb, 4(C H2 N1.5)

PLAT242_ALERT_2_C Low ’MainMol’ Ueq as Compared to Neighbors of Pb1 Check

PLAT242_ALERT_2_C Low ’MainMol’ Ueq as Compared to Neighbors of N1 Check

PLAT260_ALERT_2_C Large Average Ueq of Residue Including N1 0.105 Check

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 8 Report

0 2 0, 0 4 0, 2 0 4, 0 0 10, 0 0 12, 0 0 14,

0 0 16, 0 2 16,

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 1 Report

H1A

PLAT013_ALERT_1_G N.O.K. _shelx_hkl_checksum Found in CIF ..... Please Check

PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as mixed Check

PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records 1 Report

PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 1 Report

PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 1 Report

PLAT300_ALERT_4_G Atom Site Occupancy of N2 Constrained at 0.5 Check

PLAT300_ALERT_4_G Atom Site Occupancy of C2 Constrained at 0.5 Check

PLAT300_ALERT_4_G Atom Site Occupancy of H1A Constrained at 0.5 Check

PLAT300_ALERT_4_G Atom Site Occupancy of H1B Constrained at 0.5 Check

PLAT300_ALERT_4_G Atom Site Occupancy of H2 Constrained at 0.5 Check

PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 2) 57% Note

PLAT794_ALERT_5_G Tentative Bond Valency for Pb1 (II) . 2.68 Info

PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 15 Note

PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !

PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note

0 0 2,

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 17 Note

PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 10 Note

0 0 10, 0 0 12, 0 0 14, 0 0 16, 0 2 0, 0 2 16,

0 4 0, 2 0 4, 4 6 22, 5 3 25,

PLAT961_ALERT_5_G Dataset Contains no Negative Intensities ..... Please Check

PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 2.09 Note

Predicted wR2: Based on SigI**2 2.51 or SHELX Weight 5.21

---

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

21 **ALERT level G** = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

4 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
9 ALERT type 4 Improvement, methodology, query or suggestion

5 ALERT type 5 Informative message, check

Datablock: triag2pbcl4_i_370_00

Bond precision: N- C = 0.0100 A			Wavelength=0.71073
Cell:	a=7.5639(2)	b=8.2984(2)	c=21.7768(7)
	alpha=90	beta=90	gamma=90
Temperature:	370 K		
	Calculated		Reported
Volume	1366.89(7)		1366.89(7)
Space group	F m m m		F m m m
Hall group	-F 2 2		-F 2 2
Moiety formula 4(Cl Pb0.25), 2(C2 H4 N3) Cl4 Pb, 4(C H2 N1.5)			
Sum formula	C4 H8 Cl4 N6 Pb		C4 H8 Cl4 N6 Pb
Mr	489.16		489.15
Dx,g cm-3	2.377		2.377
Z	4		4
Mu (mm-1)	13.104		13.104
F000	896.0		896.0
F000’	885.70		
h,k,lmax	10,11,29		10,11,29
Nref	537		515
Tmin,Tmax	0.109,0.208		0.043,0.194

Tmin' 0.001

Correction method= # Reported T Limits: Tmin=0.043 Tmax=0.194

AbsCorr = ANALYTICAL

Data completeness= 0.959 Theta(max)= 29.009

wR2(reflections)= R(reflections)= 0.0219(515)

0.0466(515)

S = 1.085 Npar= 30

The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level**. Click on the hyperlinks for more details of the test.

Alert level C

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check

Calc: 4(Cl Pb0.25), 2(C2 H4 N3)

Rep.: Cl4 Pb, 4(C H2 N1.5)

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Pb1 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N1 Check

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 6 Report

0 2 0, 2 0 4, 0 0 6, 0 0 8, 0 0 10, 0 0 14,

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 2 Report

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 1 Report

H1A

PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum Found in CIF ..... Please Check

PLAT013_ALERT_1_G N.O.K. _shelx_hkl_checksum Found in CIF ..... Please Check

PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as mixed Check

PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records 1 Report

PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 1 Report

PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report

PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 1 Report

PLAT300_ALERT_4_G Atom Site Occupancy of N2 Constrained at 0.5 Check

PLAT300_ALERT_4_G Atom Site Occupancy of C2 Constrained at 0.5 Check

PLAT300_ALERT_4_G Atom Site Occupancy of H1A Constrained at 0.5 Check

PLAT300_ALERT_4_G Atom Site Occupancy of H1B Constrained at 0.5 Check

PLAT300_ALERT_4_G Atom Site Occupancy of H2 Constrained at 0.5 Check

PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 2) 57% Note

PLAT794_ALERT_5_G Tentative Bond Valency for Pb1 (II) . 2.72 Info

PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 27 Note

PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !

PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note

0 0 2,

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 15 Note

PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 7 Note

0 0 6, 0 0 8, 0 0 10, 0 0 14, 0 2 0, 1 5 25,

2 0 4,

PLAT940_ALERT_3_G Fsqd Refinement With I > n * Sigma(I) Only ..... Please Check

PLAT961_ALERT_5_G Dataset Contains no Negative Intensities ..... Please Check

PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 2.12 Note

Predicted wR2: Based on SigI**2 2.20 or SHELX Weight 4.43

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0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

25 **ALERT level G** = General information/check it is not something unexpected

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data 4 ALERT type 2 Indicator that the structure model may be wrong or deficient

5 ALERT type 3 Indicator that the structure quality may be low

10 ALERT type 4 Improvement, methodology, query or suggestion

5 ALERT type 5 Informative message, check

Datablock: triag2pbcl4_ii_360_00

Bond precision: N- C = 0.0070 A Wavelength=0.71073

Cell: a=8.2929(2) b=7.5535(2) c=21.7496(7)

alpha=90 beta=90 gamma=90

Temperature: 360 K

	Calculated	Reported
Volume	1362.40(7)	1362.40(7)
Space group	C m c m	C m c m
Hall group	-C 2c 2	-C 2c 2
Moiety formula	Cl4 Pb, 2(C2 H4 N3)	Cl4 Pb, 2(C2 H4 N3)
Sum formula	C4 H8 Cl4 N6 Pb	C4 H8 Cl4 N6 Pb
Mr	489.16	489.15
Dx,g cm-3	2.385	2.385
Z	4	4
Mu (mm-1)	13.148	13.148
F000	896.0	896.0
F000’	885.70	

h,k,lmax	11,10,29	11,10,29
Nref	1002	957
Tmin,Tmax	0.108,0.206	0.041,0.194
Tmin'	0.001	

Correction method= # Reported T Limits: Tmin=0.041 Tmax=0.194

AbsCorr = ANALYTICAL

Data completeness= 0.955 Theta(max)= 29.073

R(reflections)= 0.0233(729) wR2(reflections)= 0.0502(957)

S = 1.131 Npar= 43

The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level**. Click on the hyperlinks for more details of the test.

Alert level B

PLAT110_ALERT_2_B ADDSYM Detects Potential Lattice Translation ... ? Check

Author Response: The symmetry has been thoroughly inspected by the presence of systemat

PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem A 100 %Fit

Author Response: Look PLAT110

PLAT113_ALERT_2_B ADDSYM Suggests Possible Pseudo/New Space Group Fmmm Check

WARNING: Disordered Atoms Excluded from Analysis

Check Model Parameter Symmetry for Reflection Data Support

Author Response: Look PLAT110

Alert level C

PLAT242_ALERT_2_C Low ’MainMol’ Ueq as Compared to Neighbors of Pb1 Check

PLAT242_ALERT_2_C Low ’MainMol’ Ueq as Compared to Neighbors of N1 Check

PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -0.017 Report

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 11 Report

2 0 0, 3 1 0, 4 0 0, 1 1 2, 0 2 3, 1 1 4,
3 1 4, 0 0 6, 1 1 7, 0 0 10, 0 0 16,

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 1 Report

H1A

PLAT013_ALERT_1_G N.O.K. _shelx_hkl_checksum Found in CIF ..... Please Check

PLAT093_ALERT_1_G No s.u.’s on H-positions, Refinement Reported as mixed Check

PLAT116_ALERT_2_G ADDSYM Included (Pseudo) Lattice Translation ... Please Check

PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records 1 Report

PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 1 Report

PLAT300_ALERT_4_G Atom Site Occupancy of N2 Constrained at 0.5 Check

PLAT300_ALERT_4_G Atom Site Occupancy of C2 Constrained at 0.5 Check

PLAT300_ALERT_4_G Atom Site Occupancy of H1A Constrained at 0.5 Check

PLAT300_ALERT_4_G Atom Site Occupancy of H1B Constrained at 0.5 Check

PLAT300_ALERT_4_G Atom Site Occupancy of H2 Constrained at 0.5 Check

PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 2) 40% Note

PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.11 Ratio

PLAT794_ALERT_5_G Tentative Bond Valency for Pb1 (II) . 2.73 Info

PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !

PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note

1 1 0, 0 0 2,

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 30 Note

PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 12 Note

0 0 6, 0 0 10, 0 0 16, 0 2 3, 1 1 0, 1 1 2,
1 1 4, 1 1 7, 2 0 0, 3 1 0, 3 1 4, 4 0 0,

PLAT955_ALERT_1_G Reported (CIF) and Actual (FCF) Lmax Differ by . 1 Units
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 2.09 Note

Predicted wR2: Based on SigI**2 2.41 or SHELX Weight 4.54

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0 **ALERT level A** = Most likely a serious problem - resolve or explain

3 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
22 **ALERT level G** = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

7 ALERT type 2 Indicator that the structure model may be wrong or deficient

4 ALERT type 3 Indicator that the structure quality may be low

10 ALERT type 4 Improvement, methodology, query or suggestion

4 ALERT type 5 Informative message, check

Datablock: triag2pbcl4_ii_340_00

Bond precision: N- C = 0.0130 A Wavelength=0.71073

Cell: a=8.2959(15) b=7.4918(15) c=21.829(6)

alpha=90 beta=90 gamma=90

Temperature: 340 K

	Calculated	Reported
Volume	1356.7(5)	1356.7(5)
Space group	C m c m	C m c m

Hall group	-C 2c 2	-C 2c 2
Moiety formula	Cl4 Pb, 2(C2 H4 N3)	Cl4 Pb, 2(C2 H4 N3)
Sum formula	C4 H8 Cl4 N6 Pb	C4 H8 Cl4 N6 Pb
Mr	489.16	489.15
Dx,g cm-3	2.395	2.395
Z	4	4
Mu (mm-1)	13.203	13.203
F000	896.0	896.0
F000’	885.70	
h,k,lmax	11,10,29	11,10,29
Nref	986	905
Tmin,Tmax	0.107,0.205	0.059,0.255
Tmin’	0.001	

Correction method= # Reported T Limits: Tmin=0.059 Tmax=0.255

AbsCorr = ANALYTICAL

Data completeness= 0.918 Theta(max)= 28.889 wR2(reflections)= 0.0913(905)

R(reflections)= 0.0343(765)

S = 1.151 Npar= 44

The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level**. Click on the hyperlinks for more details of the test.

Alert level B

PLAT110_ALERT_2_B ADDSYM Detects Potential Lattice Translation ... ? Check

Author Response: The symmetry has been thoroughly inspected by the presence of systemat

PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem A 100 %Fit

Author Response: Look PLAT110

PLAT113_ALERT_2_B ADDSYM Suggests Possible Pseudo/New Space Group Fmmm Check

WARNING: Disordered Atoms Excluded from Analysis

Check Model Parameter Symmetry for Reflection Data Support

Author Response: Look PLAT110

Alert level C

PLAT222_ALERT_3_C NonSolvent Resd 2 H Uiso(max)/Uiso(min) Range 7.6 Ratio

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Pb1 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N1 Check

PLAT260_ALERT_2_C Large Average Ueq of Residue Including N1 0.107 Check

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 9 Report

2 0 0, 2 2 0, 4 0 0, 6 2 0, 3 1 1, 5 1 1,

4 0 2, 1 1 4, 0 0 6,

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.82Ang From Pb1 -2.03 eA-3

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.91Ang From Pb1 -1.99 eA-3

PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on Pb1 1.16 eA-3

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 1 Report

H1A

PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum Found in CIF ..... Please Check

PLAT013_ALERT_1_G N.O.K. _shelx_hkl_checksum Found in CIF ..... Please Check

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 9.59 Why ?

PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as mixed Check

PLAT116_ALERT_2_G ADDSYM Included (Pseudo) Lattice Translation ... Please Check

PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records 1 Report

PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of N2 Constrained at 0.5 Check

PLAT300_ALERT_4_G Atom Site Occupancy of C2 Constrained at 0.5 Check

PLAT300_ALERT_4_G Atom Site Occupancy of H1A Constrained at 0.5 Check

PLAT300_ALERT_4_G Atom Site Occupancy of H1B Constrained at 0.5 Check

PLAT300_ALERT_4_G Atom Site Occupancy of H2 Constrained at 0.5 Check

PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 2) 40% Note

PLAT650_ALERT_4_G SWAT Instruction Used to Model Solvent Disorder ! Report

PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.11 Ratio

PLAT794_ALERT_5_G Tentative Bond Valency for Pb1 (II) . 2.76 Info

PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !

PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 3 Note

1 1 0, 0 0 2, 0 0 4,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 67 Note

PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 2 Note

2 2 0, 0 0 6,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 13 Note

0 0 4, 0 0 6, 0 10 1, 1 1 0, 1 1 4, 2 0 0,

2 2 0, 3 1 1, 4 0 0, 4 0 2, 5 1 1, 6 2 0,

7 7 8,

PLAT955_ALERT_1_G Reported (CIF) and Actual (FCF) Lmax Differ by . 1 Units

PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 3.46 Note

Predicted wR2: Based on SigI**2 2.64 or SHELX Weight 8.13

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0 **ALERT level A** = Most likely a serious problem - resolve or explain

3 **ALERT level B** = A potentially serious problem, consider carefully

8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

26 **ALERT level G** = General information/check it is not something unexpected

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

12 ALERT type 2 Indicator that the structure model may be wrong or deficient

5 ALERT type 3 Indicator that the structure quality may be low

11 ALERT type 4 Improvement, methodology, query or suggestion

4 ALERT type 5 Informative message, check

Datablock: triag2pbcl4_iii_320_00

Bond precision: N- N = 0.0090 A		Wavelength=0.71073	
Cell:	a=7.5195(2)	b=21.5921(7)	c=8.3020(2)
	alpha=90	beta=90	gamma=90
Temperature:	320 K		

	1347.93(7)	1347.93(7)
	P n m a	P n m a
	-P 2ac 2n	-P 2ac 2n
Moiety formula	Cl4 Pb, 2(C2 H4 N3)	Cl4 Pb, 2(C2 H4 N3)
Sum formula	C4 H8 Cl4 N6 Pb	C4 H8 Cl4 N6 Pb
Mr	489.16	489.15
Dx,g cm-3	2.411	2.410
Z	4	4
Mu (mm-1)	13.289	13.289
F000	896.0	896.0
F000’	885.70	
h,k,lmax	10,29,11	10,29,11
Nref	1872	1768
Tmin,Tmax	0.022,0.148	0.040,0.190
Tmin’	0.000	

Correction method= # Reported T Limits: Tmin=0.040 Tmax=0.190

AbsCorr = ANALYTICAL

Data completeness= 0.944 Theta(max)= 29.160

wR2(reflections)= 0.0515(1768)

R(reflections)= 0.0266(1180)

S = 1.118 Npar= 78

The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level**. Click on the hyperlinks for more details of the test.

Alert level A

PLAT027_ALERT_3_A _diffrn_reflns_theta_full value (too) Low ..... 20.00 Degree

Author Response: This data comes from high-temperature measurements which inflicted the

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Alert level C

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.978 Why?

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Pb1 Check

PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -0.030 Report

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 12 Report

0 10 0, 0 14 0, 0 3 1, 3 3 1, 0 5 1, 0 7 1,

3 7 1, 0 0 2, 3 1 3, 3 7 3, 0 0 4, 0 2 4,

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 2.14Ang From Cl1 1.76 eA-3

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 2 Report

H1 H2

PLAT063_ALERT_4_G Crystal Size Possibly too Large for Beam Size .. 0.62 mm

PLAT794_ALERT_5_G Tentative Bond Valency for Pb1 (II) . 2.63 Info

PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info

PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !

PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note

0 2 0, 0 1 1,

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 90 Note

PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 13 Note

0 0 2, 0 0 4, 0 1 1, 0 2 4, 0 3 1, 0 5 1,

0 7 1, 0 10 0, 0 14 0, 3 1 3, 3 3 1, 3 7 1,

3 7 3,

PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 2.04 Note

Predicted wR2: Based on SigI**2 2.52 or SHELX Weight 4.71

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1 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

10 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

3 ALERT type 2 Indicator that the structure model may be wrong or deficient

5 ALERT type 3 Indicator that the structure quality may be low

3 ALERT type 4 Improvement, methodology, query or suggestion
4 ALERT type 5 Informative message, check

Datablock: triag2pbcl4_iii_300_00

Bond precision: N- C = 0.0085 A Wavelength=0.71073

Cell:	a=7.4929(3)	b=21.5667(10)	c=8.3106(4)
	alpha=90	beta=90	gamma=90
Temperature:	300 K		
	1342.97(10)	1342.97(10)	
	P n m a	P n m a	
	-P 2ac 2n	-P 2ac 2n	
Moiety formula	Cl4 Pb, 2(C2 H4 N3)	Cl4 Pb, 2(C2 H4 N3)	
Sum formula	C4 H8 Cl4 N6 Pb	C4 H8 Cl4 N6 Pb	
Mr	489.16	489.15	
Dx,g cm-3	2.419	2.419	
Z	4	4	
Mu (mm-1)	13.338	13.338	
F000	896.0	896.0	
F000’	885.70		
h,k,lmax	10,29,11	10,28,11	
Nref	1823	1675	
Tmin,Tmax	0.104,0.202	0.059,0.248	
Tmin’	0.001		

Correction method= # Reported T Limits: Tmin=0.059 Tmax=0.248

AbsCorr = ANALYTICAL

Data completeness= 0.919 Theta(max)= 28.953

wR2(reflections)=

R(reflections)= 0.0275(1299)

0.0656(1675)

S = 1.114 Npar= 78

The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level**. Click on the hyperlinks for more details of the test.

Alert level C

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Pb1 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 4.050 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.001 Check

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 21 Report

8 2 0, 0 4 0, 0 6 0, 0 8 0, 0 10 0, 0 3 1,

0 5 1, 5 6 1, 0 7 1, 0 0 2, 8 0 2, 8 4 2,

8 6 2, 8 8 2, 1 0 3, 1 1 3, 0 0 4, 0 2 4,

8 4 4, 3 0 5, 1 1 5,

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 2 Report

H1 H2

PLAT794_ALERT_5_G Tentative Bond Valency for Pb1 (II) . 2.62 Info

PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !

PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note

0 2 0, 0 1 1,

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 123 Note

PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 2 Note

0 6 0, 0 8 0,

PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 22 Note

0 0 2, 0 0 4, 0 1 1, 0 2 4, 0 3 1, 0 4 0,

0 5 1, 0 7 1, 0 8 0, 0 10 0, 1 0 3, 1 1 3,
1 1 5, 3 0 5, 3 0 10, 5 6 1, 8 0 2, 8 2 0,
8 4 2, 8 4 4, 8 6 2, 8 8 2,

PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 2.65 Note

Predicted wR2: Based on SigI**2 2.47 or SHELX Weight 6.03

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully

4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

9 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low

1 ALERT type 4 Improvement, methodology, query or suggestion

4 ALERT type 5 Informative message, check

Datablock: triag2pbcl4_iii_280_00

Bond precision: N- C = 0.0072 A Wavelength=0.71073

Cell:	a=7.4798(4)	b=21.5667(13)	c=8.3086(4)
	alpha=90	beta=90	gamma=90
Temperature:	280 K		
	1340.30(13)	1340.30(13)	
	P n m a	P n m a	
	-P 2ac 2n	-P 2ac 2n	
Moiety formula	Cl4 Pb, 2(C2 H4 N3)	Cl2.286 Pb0.571, 1.143(C2 H4 N3)	

Sum formula	C4 H8 Cl4 N6 Pb	C2.29 H4.57 Cl2.29 N3.43 Pb0.57
Mr	489.16	279.52
Dx,g cm-3	2.424	2.424
Z	4	7
Mu (mm-1)	13.364	13.364
F000	896.0	896.0
F000’	885.70	
h,k,lmax	10,29,11	10,28,11
Nref	1822	1662
Tmin,Tmax	0.088,0.201	0.057,0.248
Tmin’	0.001	

Correction method= # Reported T Limits: Tmin=0.057 Tmax=0.248

AbsCorr = ANALYTICAL

Data completeness= 0.912 Theta(max)= 28.970

R(reflections)= 0.0244(1339) wR2(reflections)= 0.0575(1662)

S = 1.133 Npar= 78

The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level**. Click on the hyperlinks for more details of the test.

Alert level C

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.972 Why?

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check

Calc: Cl4 Pb, 2(C2 H4 N3)

Rep.: Cl2.286 Pb0.571, 1.143(C2 H4 N3)

PLAT242_ALERT_2_C Low ’MainMol’ Ueq as Compared to Neighbors of Pb1 Check

PLAT245_ALERT_2_C U(iso) H1A Smaller than U(eq) C1 by 0.013 Ang**2

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 3.200 Check

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 33 Report

4 3 0, 0 6 0, 0 8 0, 5 0 1, 5 2 1, 0 3 1,

0 5 1, 5 6 1, 0 7 1, 5 8 1, 5 10 1, 5 14 1,

0 0 2, 8 0 2, 8 2 2, 1 0 3, 1 1 3, 5 2 3,

7 3 3, 5 4 3, 7 5 3, 5 6 3, 5 8 3, 5 10 3,

5 12 3, 5 16 3, 0 0 4, 0 2 4, 1 1 5, 5 6 5,

0 0 6, 5 2 7, 5 6 7,

Alert level G

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

CELLZ01_ALERT_1_G ALERT: check formula stoichiometry or atom site occupancies.

From the CIF: _cell_formula_units_Z 7

From the CIF: _chemical_formula_sum C2.29 H4.57 Cl2.29 N3.43 Pb0.57
TEST: Compare cell contents of formula and atom_site data

atom Z*formula cif sites diff C
16.03 16.00 0.03

H 31.99 32.00 -0.01

Cl 16.03 16.00 0.03

N 24.01 24.00 0.01

Pb 3.99 4.00 -0.01

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 2 Report

H1 H2

PLAT013_ALERT_1_G N.O.K. _shelx_hkl_checksum Found in CIF ..... Please Check

PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.571 Check

PLAT794_ALERT_5_G Tentative Bond Valency for Pb1 (II) . 2.60 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !

PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note

0 2 0,

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 124 Note

PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 2 Note

0 6 0, 0 8 0,

PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 32 Note

0 0 2, 0 0 4, 0 0 6, 0 2 4, 0 3 1, 0 5 1,

0 7 1, 0 8 0, 1 0 3, 1 1 3, 1 1 5, 4 3 0,

5 0 1, 5 2 1, 5 2 3, 5 2 7, 5 4 3, 5 6 1,

5 6 3, 5 6 5, 5 6 7, 5 8 1, 5 8 3, 5 10 1,

5 10 3, 5 12 3, 5 14 1, 5 16 3, 7 3 3, 7 5 3,

8 0 2, 8 2 2,

PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 2.63 Note

Predicted wR2: Based on SigI**2 2.19 or SHELX Weight 5.19

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0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

13 **ALERT level G** = General information/check it is not something unexpected

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data 3 ALERT type 2 Indicator that the structure model may be wrong or deficient

5 ALERT type 3 Indicator that the structure quality may be low

1 ALERT type 4 Improvement, methodology, query or suggestion

4 ALERT type 5 Informative message, check

Datablock: triag2pbcl4_iv_250_00

Bond precision: N- C = 0.0111 A Wavelength=0.71073

Cell:	a=21.4831(12)	b=8.3057(3)	c=7.4695(3)
	alpha=90	beta=90.036(4)	gamma=90
Temperature:	250 K		
	Calculated	Reported	
Volume	1332.80(10)	1332.80(10)	
Space group	P 21/c	P 1 21/c 1	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	Cl4 Pb, 2(C2 H4 N3)	Cl4 Pb, 2(C2 H4 N3)	
Sum formula	C4 H8 Cl4 N6 Pb	C4 H8 Cl4 N6 Pb	
Mr	489.16	489.15	
Dx,g cm-3	2.438	2.438	
Z	4	4	
Mu (mm-1)	13.440	13.440	
F000	896.0	896.0	
F000’	885.70		
h,k,lmax	29,11,10	28,11,10	
Nref	3553	3182	
Tmin,Tmax	0.102,0.199	0.134,1.000	
Tmin’	0.001		

Correction method= # Reported T Limits: Tmin=0.134 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 0.896 Theta(max)= 29.030

R(reflections)= 0.0354(2395) wR2(reflections)= 0.0906(3182)

S = 1.251 Npar= 138

The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level**. Click on the hyperlinks for more details of the test.

Alert level B

PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem n 100 %Fit

Author Response: The symmetry has been thoroughly inspected by the presence of systemat

PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem m 100 %Fit

Author Response: The symmetry has been thoroughly inspected by the presence of systemat

PLAT113_ALERT_2_B ADDSYM Suggests Possible Pseudo/New Space Group Pnma Check

Check Model Parameter Symmetry for Reflection Data Support

Author Response: look PLAT112

PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 5 Check

8 0 0, 4 1 0, 1 2 0, 3 2 0, 5 2 0,

Author Response: Some of the reflection with high errors were omitted

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Alert level C

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Pb1 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 22.355 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.598 Check

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.78Ang From Pb1 1.98 eA-3

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.73Ang From Pb1 1.96 eA-3

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.02Ang From Pb1 -1.61 eA-3

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.97Ang From Pb1 -1.52 eA-3

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 4 Report

H1A H2A H1B H2B

PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum Found in CIF ..... Please Check

PLAT013_ALERT_1_G N.O.K. _shelx_hkl_checksum Found in CIF ..... Please Check

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 4 Note

H1AA H1BA H2AA H2BA

PLAT794_ALERT_5_G Tentative Bond Valency for Pb1 (II) . 2.60 Info

PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !

PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note

1 0 0, 2 0 0,

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 364 Note

PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 1 Note

6 0 0,

PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 4.6 Low

PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 2.64 Note

Predicted wR2: Based on SigI**2 3.43 or SHELX Weight 7.40

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0 **ALERT level A** = Most likely a serious problem - resolve or explain

4 **ALERT level B** = A potentially serious problem, consider carefully

7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

13 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data 8
ALERT type 2 Indicator that the structure model may be wrong or deficient

6 ALERT type 3 Indicator that the structure quality may be low

3 ALERT type 4 Improvement, methodology, query or suggestion
4 ALERT type 5 Informative message, check

Datablock: triag2pbcl4_iv_220_00

Bond precision: N- C = 0.0105 A		Wavelength=0.71073	
Cell:	a=21.4566(15)	b=8.3029(3)	c=7.4446(3)
	alpha=90	beta=90.036(4)	gamma=90
Temperature:	220 K		
	Calculated	Reported	
Volume	1326.27(12)	1326.27(12)	
Space group	P 21/c	P 1 21/c 1	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	Cl4 Pb, 2(C2 H4 N3)	Cl4 Pb, 2(C2 H4 N3)	
Sum formula	C4 H8 Cl4 N6 Pb	C4 H8 Cl4 N6 Pb	
Mr	489.16	489.15	
Dx,g cm-3	2.450	2.450	
Z	4	4	
Mu (mm-1)	13.506	13.506	
F000	896.0	896.0	
F000’	885.70		
h,k,lmax	29,11,10	28,11,10	
Nref	3538	3158	
Tmin,Tmax	0.101,0.198	0.144,1.000	
Tmin’	0.001		

Correction method= # Reported T Limits: Tmin=0.144 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 0.893 Theta(max)= 29.054

R(reflections)= 0.0402(2441) wR2(reflections)= 0.0931(3145)

S = 1.110 Npar= 77

The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level**. Click on the hyperlinks for more details of the test.

Alert level B

PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem n 100 %Fit

Author Response: The symmetry has been thoroughly inspected by the presence of systemat

PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem m 100 %Fit **Author Response: The symmetry has been thoroughly inspected by the presence of systemat**

PLAT113_ALERT_2_B ADDSYM Suggests Possible Pseudo/New Space Group Pnma Check

Check Model Parameter Symmetry for Reflection Data Support

Author Response: look PLAT112

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.88Ang From Pb1 -2.75 eA-3

Author Response: Residual density near heavy atom.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.97Ang From Pb1 -2.71 eA-3

Author Response: Residual density near heavy atom.

Alert level C

PLAT218_ALERT_3_C Constrained U(ij) Components(s) for N2A . 6 Check

PLAT218_ALERT_3_C Constrained U(ij) Components(s) for N1B . 6 Check

PLAT218_ALERT_3_C Constrained U(ij) Components(s) for N1A . 6 Check

PLAT218_ALERT_3_C Constrained U(ij) Components(s) for N2B . 6 Check

PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C1A . 6 Check

PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C1B . 6 Check

PLAT218_ALERT_3_C Constrained U(ij) Components(s) for N3A . 6 Check

PLAT218_ALERT_3_C Constrained U(ij) Components(s) for N3B . 6 Check

PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C2A . 6 Check

PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C2B . 6 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Pb1 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 31.137 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 3.150 Check

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 14 Report

0 2 0, 1 2 0, 3 0 0, 3 1 0, 3 2 0, 3 4 0,

4 1 0, 4 3 0, 5 1 0, 5 2 0, 6 0 0, 7 2 0,

8 0 0, 0 3 1,

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.94Ang From Pb1 1.87 eA-3

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.88Ang From Pb1 1.59 eA-3

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.91Ang From Pb1 1.57 eA-3

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.92Ang From Pb1 1.55 eA-3

PLAT992_ALERT_5_C Repd & Actual _reflns_number_gt Values Differ by 14 Check

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Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 10 Note

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 4 Report

H1A H2A H1B H2B

PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum Found in CIF ..... Please Check

PLAT013_ALERT_1_G N.O.K. _shelx_hkl_checksum Found in CIF ..... Please Check

PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 5 Report

PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 3 Report

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 4 Note

H1AA H1BA H2AA H2BA

PLAT794_ALERT_5_G Tentative Bond Valency for Pb1 (II) . 2.60 Info

PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info

PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 61 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !

PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note

1 0 0, 2 0 0,

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 374 Note

PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 1 Note

6 0 0,

PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 13 Note

0 2 0, 0 3 1, 1 2 0, 3 0 0, 3 1 0, 3 2 0,

3 4 0, 4 1 0, 4 3 0, 5 1 0, 5 2 0, 7 2 0,

8 0 0,

PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 4.6 Low

PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 2.88 Note

Predicted wR2: Based on SigI**2 3.23 or SHELX Weight 8.49

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0 **ALERT level A** = Most likely a serious problem - resolve or explain

5 **ALERT level B** = A potentially serious problem, consider carefully

19 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

18 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

12 ALERT type 2 Indicator that the structure model may be wrong or deficient

17 ALERT type 3 Indicator that the structure quality may be low

5 ALERT type 4 Improvement, methodology, query or suggestion

5 ALERT type 5 Informative message, check

Datablock: triag2pbcl4_iv_200_00

Bond precision: N- N = 0.0120 A Wavelength=0.71073

Cell:	a=21.4424(18)	b=8.2994(3)	c=7.4252(4)
	alpha=90	beta=90.093(5)	gamma=90

Temperature: 200 K

	Calculated	Reported
Volume	1321.38(14)	1321.38(14)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	Cl4 Pb, 2(C2 H4 N3)	Cl4 Pb, 2(C2 H4 N3)
Sum formula	C4 H8 Cl4 N6 Pb	C4 H8 Cl4 N6 Pb
Mr	489.16	489.15
Dx,g cm-3	2.459	2.459
Z	4	4
Mu (mm-1)	13.556	13.556
F000	896.0	896.0
F000’	885.70	
h,k,lmax	29,11,10	28,11,10
Nref	3486	3145
Tmin,Tmax	0.100,0.197	0.160,1.000
Tmin’	0.001	

Correction method= # Reported T Limits: Tmin=0.160 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 0.902 Theta(max)= 28.920

wR2(reflections)=

R(reflections)= 0.0419(2470)

0.0980(3127)

S = 1.155 Npar= 145

The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level**. Click on the hyperlinks for more details of the test.

Alert level B

PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem n 100 %Fit

Author Response: The symmetry has been thoroughly inspected by the presence of systemat

PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem m 100 %Fit

Author Response: The symmetry has been thoroughly inspected by the presence of systemat

PLAT113_ALERT_2_B ADDSYM Suggests Possible Pseudo/New Space Group Pnma Check

Check Model Parameter Symmetry for Reflection Data Support

Author Response: The symmetry has been thoroughly inspected by the presence of systemat

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.97Ang From Pb1 -3.30 eA-3

Author Response: Residual density near heavy atom.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.98Ang From Pb1 -3.18 eA-3

Author Response: Residual density near heavy atom.

Alert level C

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Pb1 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 41.139 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 3.139 Check

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 19 Report

0 2 0, 0 4 0, 1 2 0, 3 0 0, 3 1 0, 3 2 0,

3 4 0, 4 0 0, 4 1 0, 4 3 0, 5 1 0, 5 2 0,

6 0 0, 8 0 0, 23 3 0, 24 0 0, 24 2 1, -4 0 2,

22 1 2,

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.77Ang From Pb1 1.57 eA-3

PLAT992_ALERT_5_C Repd & Actual _reflns_number_gt Values Differ by 17 Check

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Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 10 Note

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 2 Report

H1A H1B

PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum Found in CIF ..... Please Check

PLAT013_ALERT_1_G N.O.K. _shelx_hkl_checksum Found in CIF ..... Please Check

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 5.19 Why ?

PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 5 Report

PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 3 Report

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 4 Note

H1AA H1BA H2AA H2BA

PLAT794_ALERT_5_G Tentative Bond Valency for Pb1 (II) . 2.61 Info

PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 2 Info

PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 61 Note

PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !

PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note

1 0 0, 2 0 0,

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 337 Note

PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 1 Note

6 0 0,

PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 18 Note

-4 0 2, 0 2 0, 0 4 0, 1 2 0, 3 0 0, 3 1 0,

3 2 0, 3 4 0, 4 0 0, 4 1 0, 4 3 0, 5 1 0,

5 2 0, 8 0 0, 22 1 2, 23 3 0, 24 0 0, 24 2 1,

PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 4.6 Low

PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 3.00 Note

Predicted wR2: Based on SigI**2 3.26 or SHELX Weight 8.69

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0 **ALERT level A** = Most likely a serious problem - resolve or explain

5 **ALERT level B** = A potentially serious problem, consider carefully

6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

19 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

10 ALERT type 2 Indicator that the structure model may be wrong or deficient

7 ALERT type 3 Indicator that the structure quality may be low

5 ALERT type 4 Improvement, methodology, query or suggestion

5 ALERT type 5 Informative message, check

Datablock: triag2pbcl4_iv_180_00

Bond precision: N- N = 0.0145 A Wavelength=0.71073

Cell: a=21.4212(18) b=8.2997(3) c=7.4042(3)

alpha=90 beta=90.020(5) gamma=90

Temperature: 180 K

Calculated Reported

Volume	1316.39(13)	1316.39(13)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	Cl4 Pb, 2(C2 H4 N3)	Cl4 Pb, 2(C2 H4 N3)
Sum formula	C4 H8 Cl4 N6 Pb	C4 H8 Cl4 N6 Pb
Mr	489.16	489.15
Dx,g cm-3	2.468	2.468
Z	4	4
Mu (mm-1)	13.607	13.607
F000	896.0	896.0
F000’	885.70	
h,k,lmax	29,11,10	28,11,10
Nref	3488	3117
Tmin,Tmax	0.099,0.195	0.495,0.778
Tmin’	0.001	

Correction method= # Reported T Limits: Tmin=0.495 Tmax=0.778

AbsCorr = ANALYTICAL

Data completeness= 0.894 Theta(max)= 28.972

wR2(reflections)= 0.1126(3113)

R(reflections)= 0.0484(2487)

S = 1.192 Npar= 137

The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level**. Click on the hyperlinks for more details of the test.

Alert level A

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.99Ang From Pb1 -4.38 eA-3

Author Response: Residual density near heavy atom.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.97Ang From Pb1 -4.25 eA-3

Author Response: Residual density near heavy atom.

Alert level B

PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem n 100 %Fit

Author Response: The symmetry has been thoroughly inspected by the presence of the syst

PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem m 100 %Fit

Author Response: The symmetry has been thoroughly inspected by the presence of the syst

PLAT113_ALERT_2_B ADDSYM Suggests Possible Pseudo/New Space Group Pnma Check

Check Model Parameter Symmetry for Reflection Data Support

Author Response: look PLAT112

Alert level C

PLAT213_ALERT_2_C Atom Cl1 has ADP max/min Ratio ..... 3.1 prolat

PLAT213_ALERT_2_C Atom Cl2 has ADP max/min Ratio ..... 3.1 prolat

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Pb1 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 53.385 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 3.403 Check

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 21 Report

0 2 0, 0 4 0, 1 2 0, 3 0 0, 3 2 0, 3 4 0,

4 0 0, 4 1 0, 5 0 0, 6 0 0, 23 0 0, 23 1 0,

23 3 0, -24 2 1, 22 2 1, 22 4 1, 24 2 1, -23 2 2,

-22 1 2, 22 3 2, -22 2 3,

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.81Ang From Pb1 1.67 eA-3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 10 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 4 Report

H1A H2A H1B H2B

PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum Found in CIF ..... Please Check

PLAT013_ALERT_1_G N.O.K. _shelx_hkl_checksum Found in CIF ..... Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 11.72 Why ?

PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 5 Report

PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 3 Report

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 4 Note

H1AA H1BA H2AA H2BA

PLAT794_ALERT_5_G Tentative Bond Valency for Pb1 (II) . 2.61 Info

PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info

PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 61 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !

PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note

1 0 0, 2 0 0,

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 350 Note

PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 1 Note

6 0 0,

PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 20 Note

-24 2 1, -23 2 2, -22 1 2, -22 2 3, 0 2 0, 0 4 0,

1 2 0, 3 0 0, 3 2 0, 3 4 0, 4 0 0, 4 1 0,

5 0 0, 22 2 1, 22 3 2, 22 4 1, 23 1 0, 23 3 0,

24 2 1, 25 3 0,

PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 4.6 Low

PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 3.68 Note

Predicted wR2: Based on SigI**2 3.05 or SHELX Weight 9.66

PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 4 Check

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2 **ALERT level A** = Most likely a serious problem - resolve or explain
3 **ALERT level B** = A potentially serious problem, consider carefully
7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

20 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data 12 ALERT type 2 Indicator that the structure model may be wrong or deficient

7 ALERT type 3 Indicator that the structure quality may be low 5 ALERT type 4 Improvement, methodology, query or suggestion

5 ALERT type 5 Informative message, check

Datablock: triag2pbcl4_iv_150_00

Bond precision: N- C = 0.0159 A		Wavelength=0.71073	
Cell:	a=21.429(2)	b=8.3075(4)	c=7.3768(4)
	alpha=90	beta=90.111(6)	gamma=90
Temperature:	150 K		
	Calculated	Reported	
Volume	1313.23(16)	1313.21(17)	
Space group	P 21/c	P 1 21/c 1	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	Cl4 Pb, 2(C2 H4 N3)	Cl4 Pb, 2(C2 H4 N3)	
Sum formula	C4 H8 Cl4 N6 Pb	C4 H8 Cl4 N6 Pb	
Mr	489.16	489.15	
Dx,g cm-3	2.474	2.474	
Z	4	4	

Mu (mm-1)	13.640	13.640
F000	896.0	896.0
F000’	885.70	
h,k,lmax	29,11,10	28,11,9
Nref	3477	3100
Tmin,Tmax	0.099,0.195	0.493,0.777
Tmin’	0.001	

Correction method= # Reported T Limits: Tmin=0.493 Tmax=0.777

AbsCorr = ANALYTICAL

Data completeness= 0.892 Theta(max)= 28.984

R(reflections)= 0.0561(2518) wR2(reflections)= 0.1259(3100)

S = 1.231 Npar= 137

The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level**. Click on the hyperlinks for more details of the test.

Alert level A

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 1.01Ang From Pb1 -5.24 eA-3

Author Response: Residual density near heavy atom.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 1.02Ang From Pb1 -5.22 eA-3

Author Response: Residual density near heavy atom.

Alert level B

PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem n 100 %Fit

Author Response: The symmetry has been thoroughly inspected by the presence of the syst

PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem m 100 %Fit

Author Response: The symmetry has been thoroughly inspected by the presence of the syst

PLAT113_ALERT_2_B ADDSYM Suggests Possible Pseudo/New Space Group Pnma Check

Check Model Parameter Symmetry for Reflection Data Support

Author Response: look PLAT112

Alert level C

PLAT213_ALERT_2_C Atom Pb1 has ADP max/min Ratio ..... 3.1 prolat

PLAT213_ALERT_2_C Atom Cl1 has ADP max/min Ratio ..... 3.2 prolat

PLAT213_ALERT_2_C Atom Cl2 has ADP max/min Ratio ..... 3.1 prolat

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Pb1 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 61.884 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 4.224 Check

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 15 Report

0 2 0, 0 4 0, 1 2 0, 4 1 0, 5 0 0, 6 0 0,

8 0 0, 21 0 0, 22 0 0, 23 0 0, 23 3 0, -24 2 1,

24 2 1, 22 1 2, -22 2 3,

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.79Ang From Pb1 1.63 eA-3

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.82Ang From Pb1 1.57 eA-3

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.06Ang From Pb1 1.52 eA-3

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.94Ang From Cl4 -1.52 eA-3

Author Response: Residual density near heavy atom.

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 10 Note

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 15 Report

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 4 Report

H1A H2A H1B H2B

PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum Found in CIF ..... Please Check

PLAT013_ALERT_1_G N.O.K. _shelx_hkl_checksum Found in CIF ..... Please Check

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 19.02 Why ?

PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 5 Report

PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 3 Report

PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 3 Report

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 4 Note

H1AA H1BA H2AA H2BA

PLAT794_ALERT_5_G Tentative Bond Valency for Pb1 (II) . 2.61 Info

PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info

PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 151 Note

PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !

PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note

1 0 0, 2 0 0,

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 348 Note

PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 1 Note

6 0 0,

PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 15 Note

-24 2 1, -24 5 2, -22 2 3, 0 2 0, 0 4 0, 1 2 0,

4 1 0, 5 0 0, 8 0 0, 22 0 0, 22 1 2, 23 3 0,

23 5 2, 24 2 1, 25 3 0,

PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 4.6 Low

PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 4.11 Note

Predicted wR2: Based on SigI**2 3.05 or SHELX Weight 10.47

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2 **ALERT level A** = Most likely a serious problem - resolve or explain
3 **ALERT level B** = A potentially serious problem, consider carefully
11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
21 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

17 ALERT type 2 Indicator that the structure model may be wrong or deficient

7 ALERT type 3 Indicator that the structure quality may be low

6 ALERT type 4 Improvement, methodology, query or suggestion

4 ALERT type 5 Informative message, check

Datablock: triag2pbcl4_iv_130_00

Bond precision: N- C = 0.0166 A Wavelength=0.71073

Cell:	a=21.423(2)	b=8.3075(4)	c=7.3587(4)
	alpha=90	beta=90.112(6)	gamma=90

Temperature: 130 K

	Calculated	Reported
Volume	1309.64(15)	1309.63(16)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	Cl4 Pb, 2(C2 H4 N3)	Cl4 Pb, 2(C2 H4 N3)
Sum formula	C4 H8 Cl4 N6 Pb	C4 H8 Cl4 N6 Pb
Mr	489.16	489.15
Dx,g cm-3	2.481	2.481

Z	4	4
Mu (mm-1)	13.677	13.677
F000	896.0	896.0
F000’	885.70	
h,k,lmax	29,11,10	28,11,9
Nref	3474	3091
Tmin,Tmax	0.098,0.194	0.492,0.777
Tmin’	0.001	

Correction method= # Reported T Limits: Tmin=0.492 Tmax=0.777

AbsCorr = ANALYTICAL

Data completeness= 0.890 Theta(max)= 29.014

R(reflections)= 0.0597(2529) wR2(reflections)= 0.1267(3091)

S = 1.255 Npar= 137

The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level**. Click on the hyperlinks for more details of the test.

Alert level A

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 1.03Ang From Pb1 -5.31 eA-3

Author Response: Residual density near heavy atom.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 1.03Ang From Pb1 -5.21 eA-3

Author Response: Residual density near heavy atom.

Alert level B

PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem n 100 %Fit

Author Response: The symmetry has been thoroughly inspected by the presence of the syst

PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem m 100 %Fit

Author Response: The symmetry has been thoroughly inspected by the presence of the syst

PLAT113_ALERT_2_B ADDSYM Suggests Possible Pseudo/New Space Group Pnma Check

Check Model Parameter Symmetry for Reflection Data Support

Author Response: look PLAT112

Alert level C

PLAT213_ALERT_2_C Atom Pb1 has ADP max/min Ratio ..... 3.3 prolat

PLAT213_ALERT_2_C Atom Cl1 has ADP max/min Ratio ..... 3.5 prolat

PLAT213_ALERT_2_C Atom Cl2 has ADP max/min Ratio ..... 3.3 prolat

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Pb1 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 65.803 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 5.351 Check

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 17 Report

0 2 0, 0 4 0, 1 2 0, 4 0 0, 4 1 0, 5 0 0,

6 0 0, 8 0 0, 23 3 0, -22 2 1, 22 4 1, 24 2 1,

21 2 2, 22 1 2, 22 3 2, -21 2 3, -21 1 4,

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.79Ang From Pb1 1.68 eA-3

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.79Ang From Pb1 1.63 eA-3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 10 Note

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 15 Report

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 4 Report

H1A H2A H1B H2B

PLAT013_ALERT_1_G N.O.K. _shelx_hkl_checksum Found in CIF ..... Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 21.06 Why ?

PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 5 Report

PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 3 Report

PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 3 Report

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 4 Note

H1AA H1BA H2AA H2BA

PLAT794_ALERT_5_G Tentative Bond Valency for Pb1 (II) . 2.61 Info

PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info

PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 151 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !

PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note

1 0 0, 2 0 0,

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 356 Note

PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 1 Note

6 0 0,

PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 19 Note

-22 2 1, -21 1 4, 0 2 0, 0 4 0, 1 2 0, 4 0 0,

4 1 0, 5 0 0, 8 0 0, 21 2 2, 22 1 2, 22 3 2,

22 4 1, 23 3 0, 23 5 2, 24 2 1, 25 3 0, 25 4 1,

28 2 1,

PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 4.6 Low

PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 4.37 Note

Predicted wR2: Based on SigI**2 2.89 or SHELX Weight 10.33

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2 **ALERT level A** = Most likely a serious problem - resolve or explain

3 **ALERT level B** = A potentially serious problem, consider carefully

9 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

20 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

15 ALERT type 2 Indicator that the structure model may be wrong or deficient

7 ALERT type 3 Indicator that the structure quality may be low

6 ALERT type 4 Improvement, methodology, query or suggestion

4 ALERT type 5 Informative message, check

Datablock: triag2pbcl4_iv_100_00

Bond precision: N- N = 0.0175 A		Wavelength=0.71073	
Cell:	a=21.419(2)	b=8.3049(4)	c=7.3363(4)
	alpha=90	beta=90.149(6)	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	1305.00(15)	1305.01(16)	
Space group	P 21/c	P 1 21/c 1	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	Cl4 Pb, 2(C2 H4 N3)	Cl4 Pb, 2(C2 H4 N3)	
Sum formula	C4 H8 Cl4 N6 Pb	C4 H8 Cl4 N6 Pb	
Mr	489.16	489.15	
Dx,g cm-3	2.490	2.490	
Z	4	4	
Mu (mm-1)	13.726	13.726	
F000	896.0	896.0	
F000’	885.70		

h,k,lmax	29,11,9	28,11,9
Nref	3386	3071
Tmin,Tmax	0.097,0.193	0.491,0.776
Tmin'	0.001	

Correction method= # Reported T Limits: Tmin=0.491 Tmax=0.776

AbsCorr = ANALYTICAL

Data completeness= 0.907 Theta(max)= 28.802

R(reflections)= 0.0641(2544) wR2(reflections)= 0.1297(3071)

S = 1.239 Npar= 137

The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level**. Click on the hyperlinks for more details of the test.

Alert level A

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 1.05Ang From Pb1 -5.43 eA-3

Author Response: Residual density near heavy atom.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 1.05Ang From Pb1 -5.35 eA-3

Author Response: Residual density near heavy atom.

Alert level B

PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem n 100 %Fit

Author Response: The symmetry has been thoroughly inspected by the presence of the syst

PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem m 100 %Fit

Author Response: The symmetry has been thoroughly inspected by the presence of the syst

PLAT113_ALERT_2_B ADDSYM Suggests Possible Pseudo/New Space Group Pnma Check Check Model Parameter Symmetry for Reflection Data Support

Author Response: look PLAT112

Alert level C

PLAT213_ALERT_2_C Atom Pb1 has ADP max/min Ratio ..... 3.8 prolat

PLAT213_ALERT_2_C Atom Cl1 has ADP max/min Ratio ..... 3.8 prolat

PLAT213_ALERT_2_C Atom Cl2 has ADP max/min Ratio ..... 3.6 prolat

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 74.682 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 5.786 Check

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 18 Report

0 2 0, 0 4 0, 1 2 0, 6 0 0, 8 0 0, -23 4 1,

-22 2 1, -21 4 1, 22 2 1, 24 2 1, -23 1 2, -22 3 2,

-1 0 2, -1 2 2, 1 0 2, 22 1 2, 22 3 2, -22 1 3,

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.64Ang From Pb1 1.95 eA-3

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.64Ang From Pb1 1.61 eA-3

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.59Ang From Pb1 1.61 eA-3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 10 Note

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 15 Report

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 4 Report

H1A H2A H1B H2B

PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum Found in CIF ..... Please Check

PLAT013_ALERT_1_G N.O.K. _shelx_hkl_checksum Found in CIF ..... Please Check

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 28.79 Why ?

PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 5 Report

PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 3 Report

PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 3 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Pb1 --Cl3 . 8.0 s.u.

PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Pb1 --Cl4 . 6.5 s.u.

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 4 Note

H1AA H1BA H2AA H2BA

PLAT794_ALERT_5_G Tentative Bond Valency for Pb1 (II) . 2.61 Info

PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info

PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 151 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !

PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note

1 0 0, 2 0 0,

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 294 Note

PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 2 Note

6 0 0, -1 2 2,

PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 26 Note

-24 3 2, -24 4 1, -24 5 2, -23 1 2, -23 1 4, -23 4 1,

-22 1 3, -22 2 1, -22 3 2, -22 4 3, -22 5 2, -21 4 1,

0 2 0, 0 4 0, 1 2 0, 8 0 0, 22 1 2, 22 2 1,

22 3 2, 23 5 2, 24 2 1, 24 3 2, 25 1 2, 25 3 0,

25 4 1, 27 3 0,

PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 4.6 Low

PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 4.51 Note

Predicted wR2: Based on SigI**2 2.87 or SHELX Weight 10.71

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2 **ALERT level A** = Most likely a serious problem - resolve or explain

3 **ALERT level B** = A potentially serious problem, consider carefully

9 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

23 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

17 ALERT type 2 Indicator that the structure model may be wrong or deficient

7 ALERT type 3 Indicator that the structure quality may be low 6 ALERT type 4 Improvement, methodology, query or suggestion

4 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

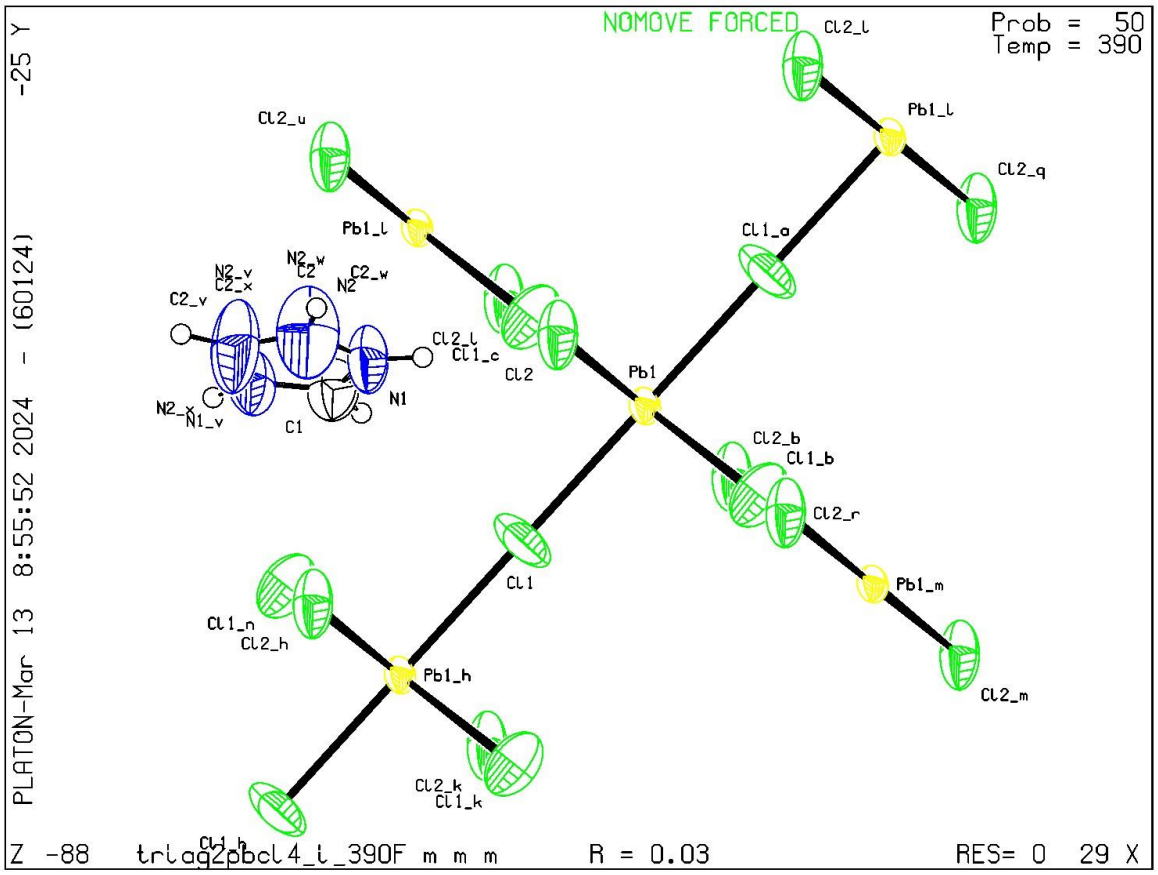
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 06/01/2024; check.def file version of 05/01/2024

Datablock triag2pbcl4_i_390_00



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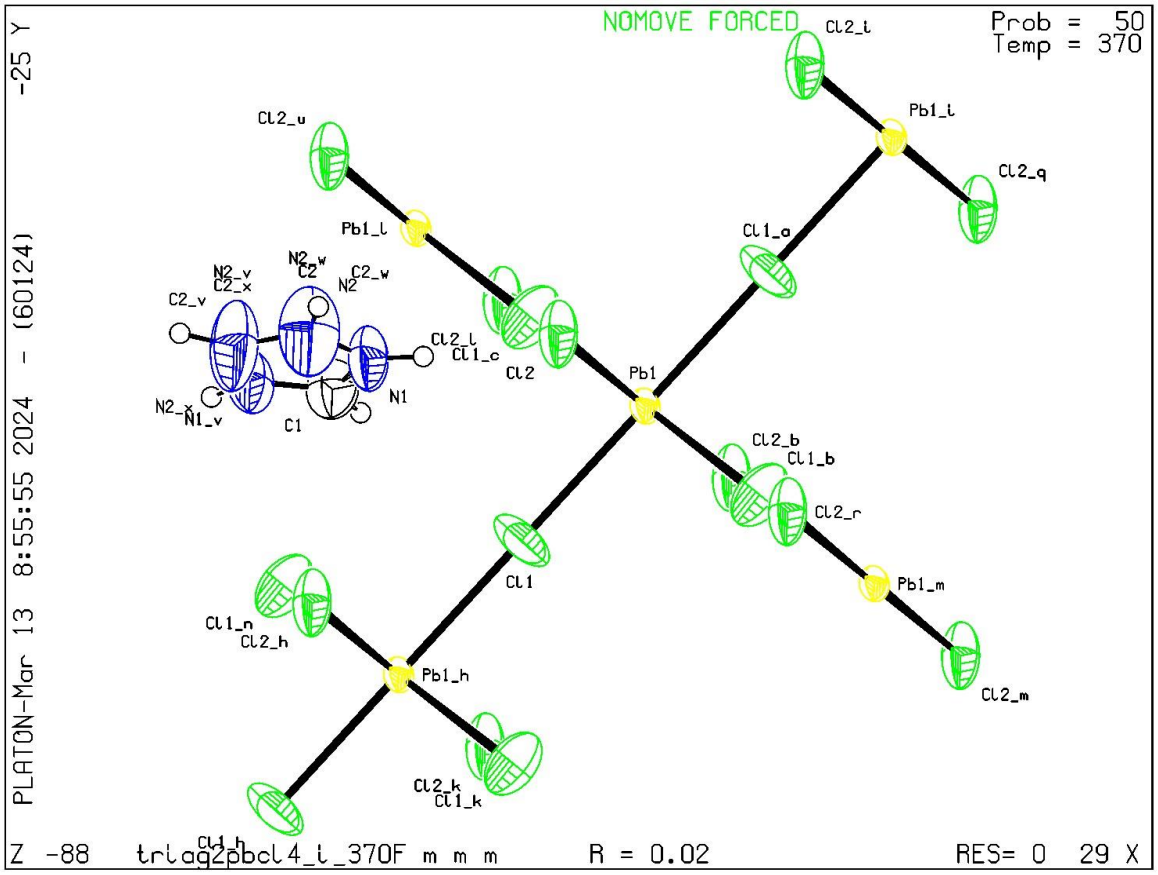

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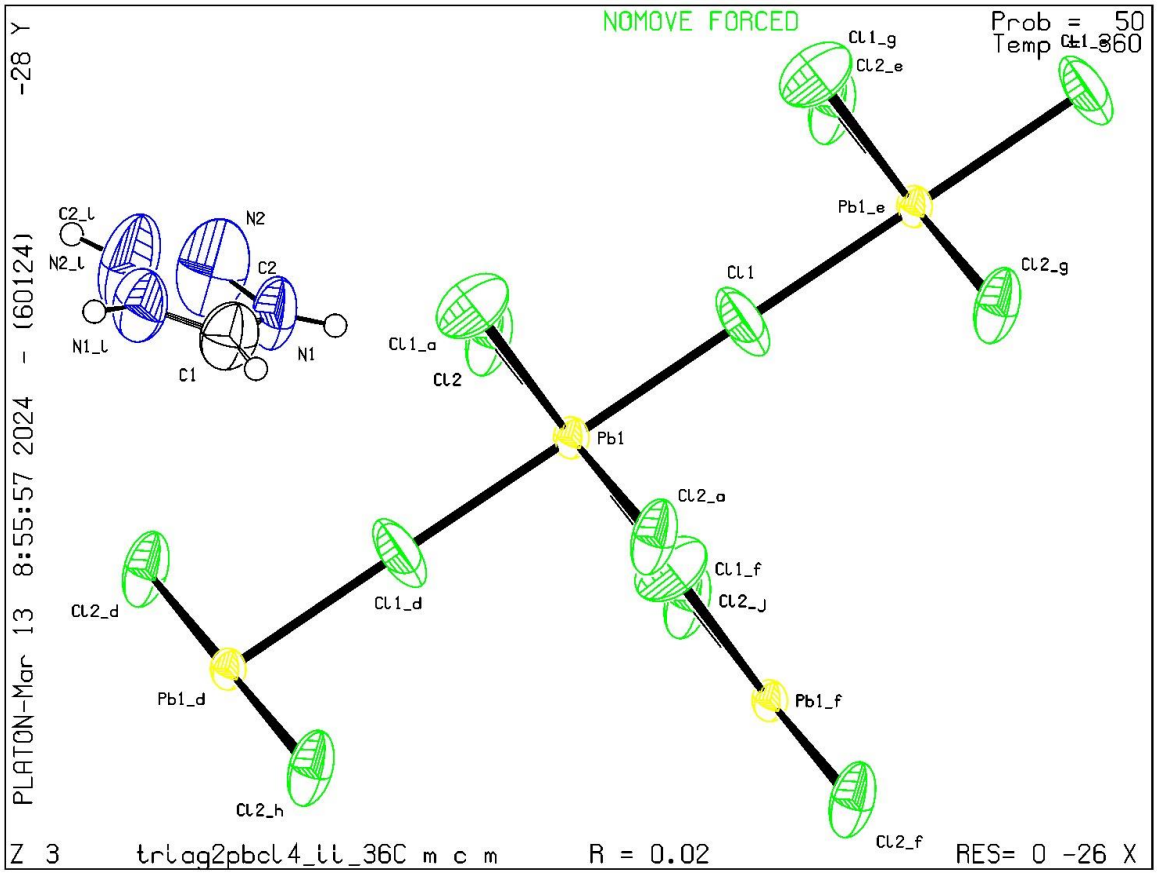

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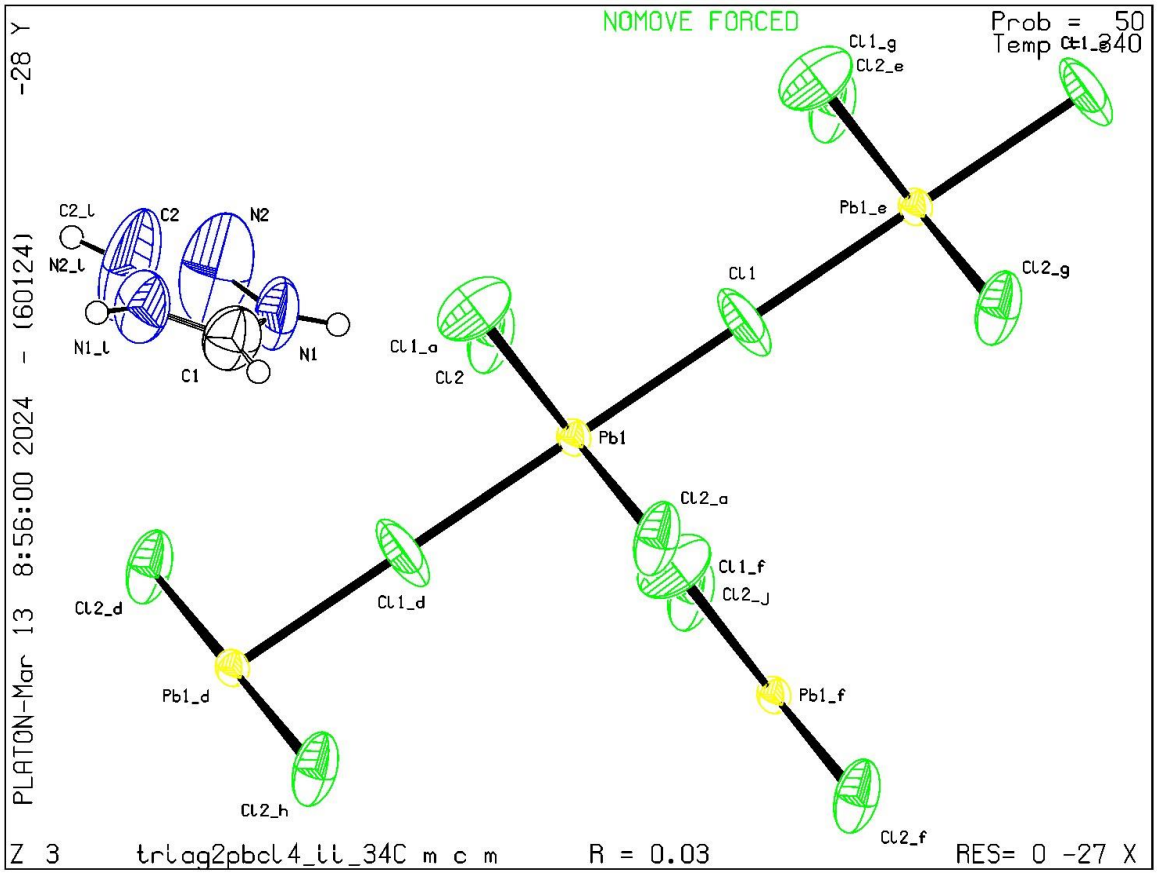

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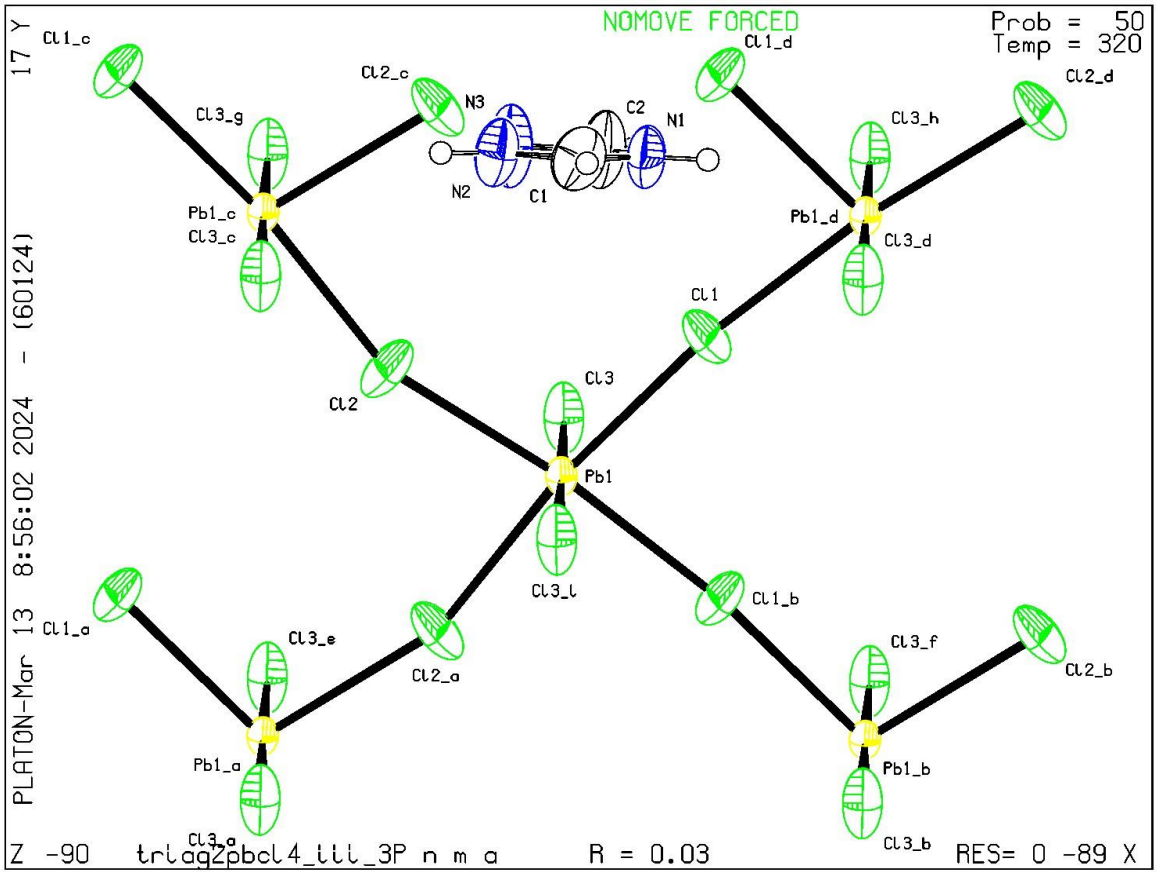

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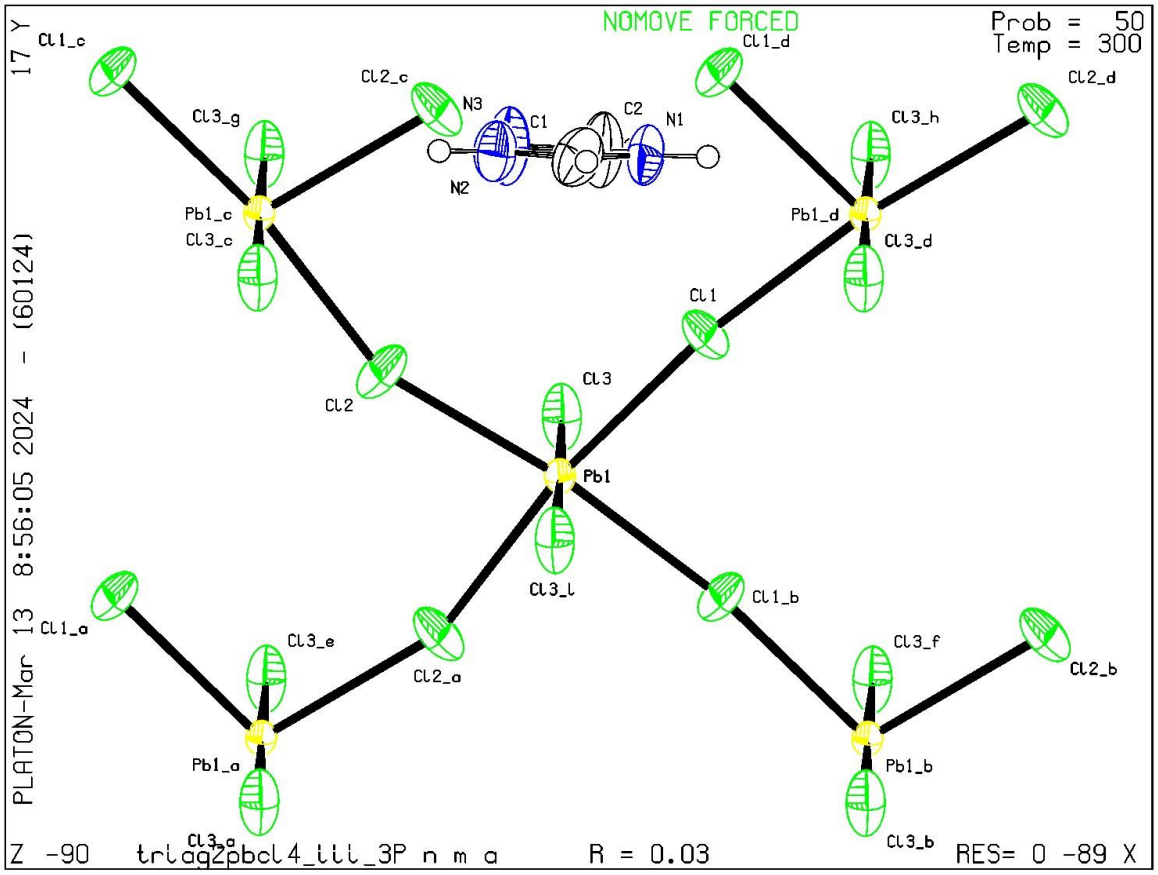

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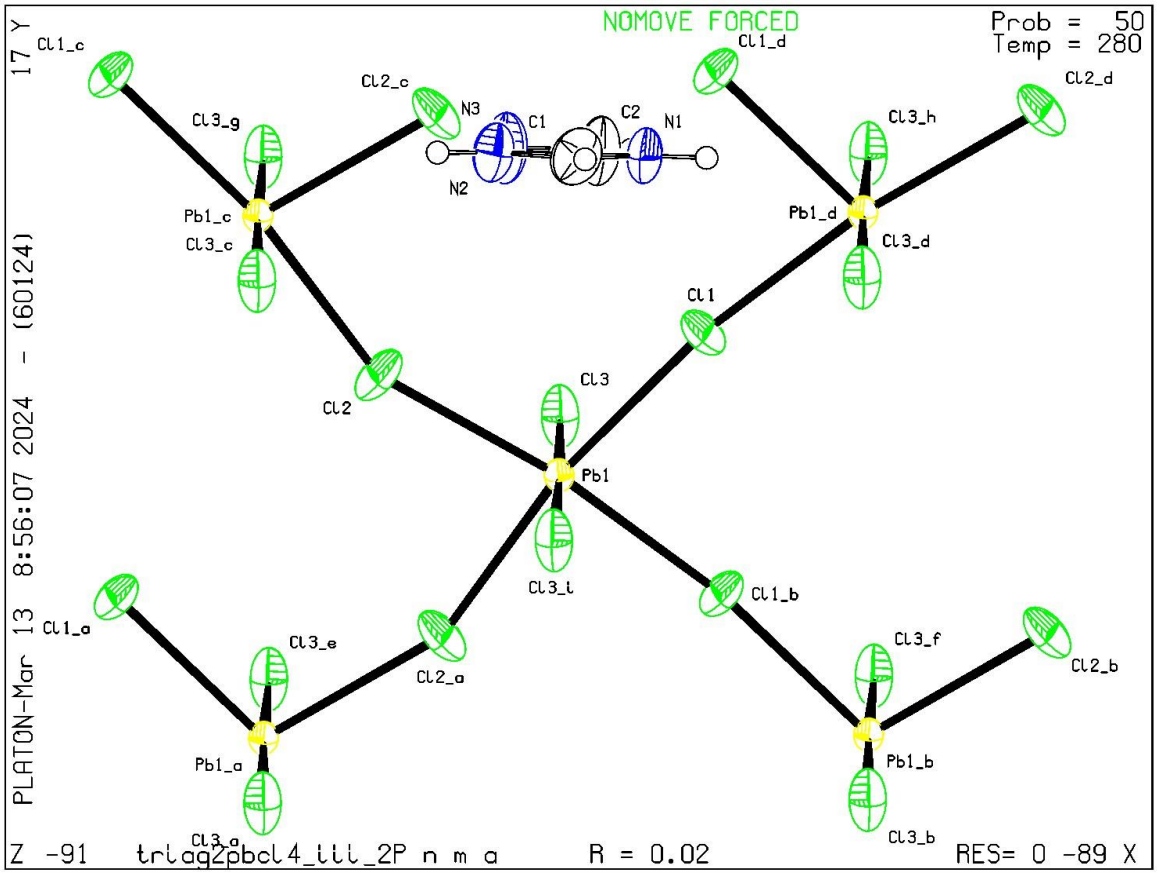

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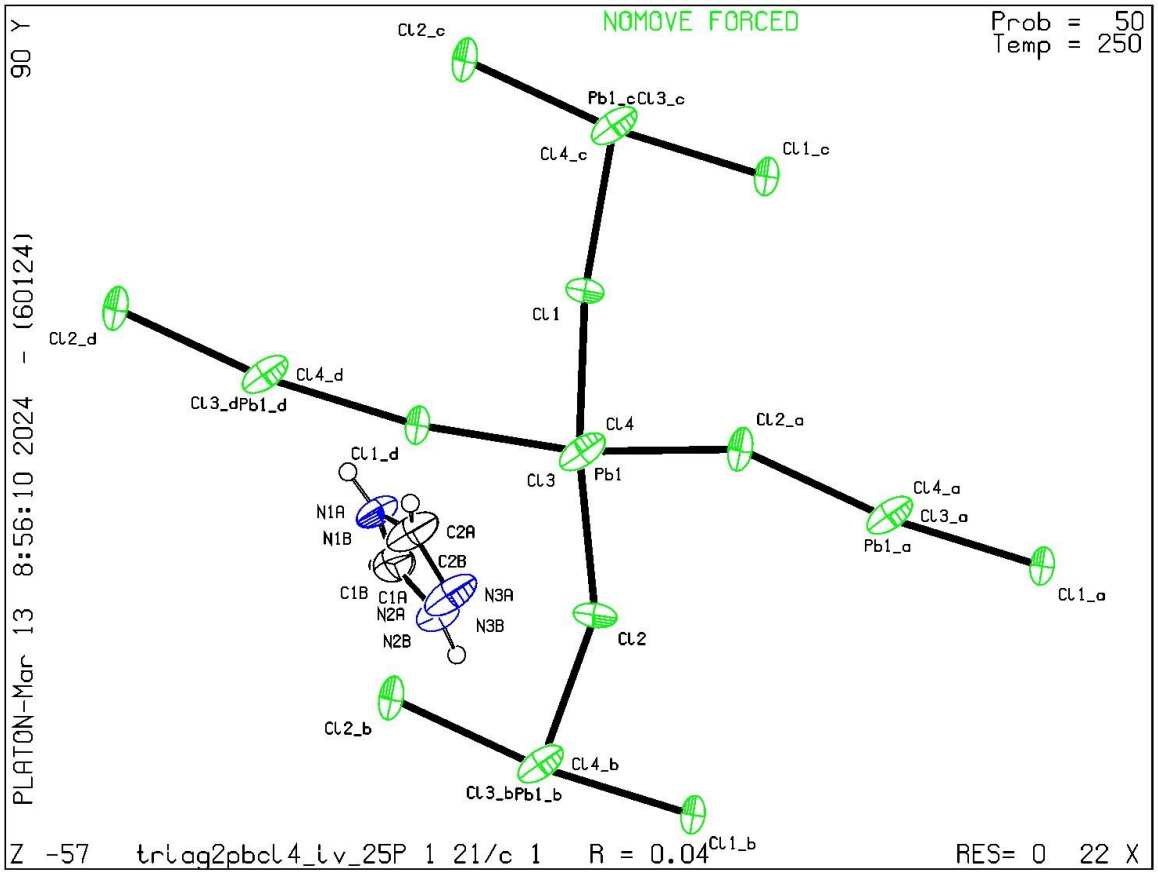

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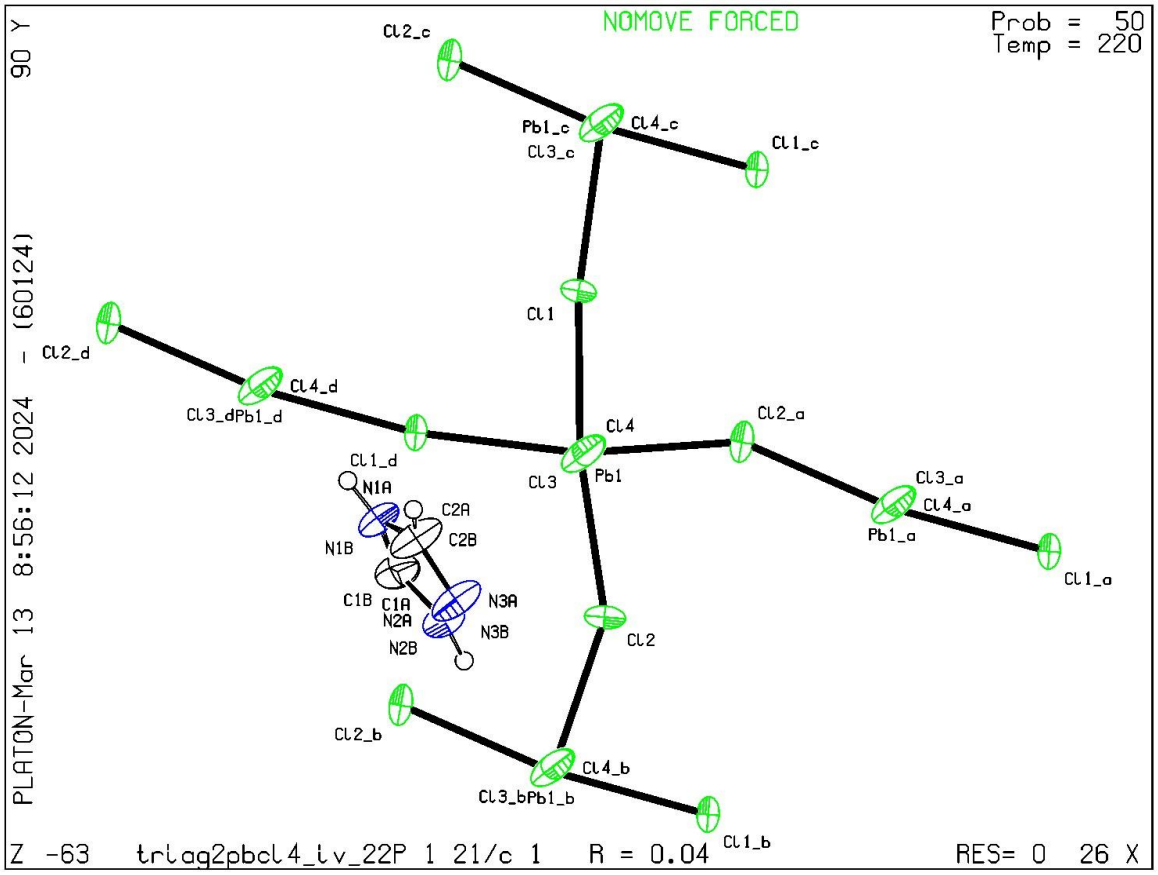

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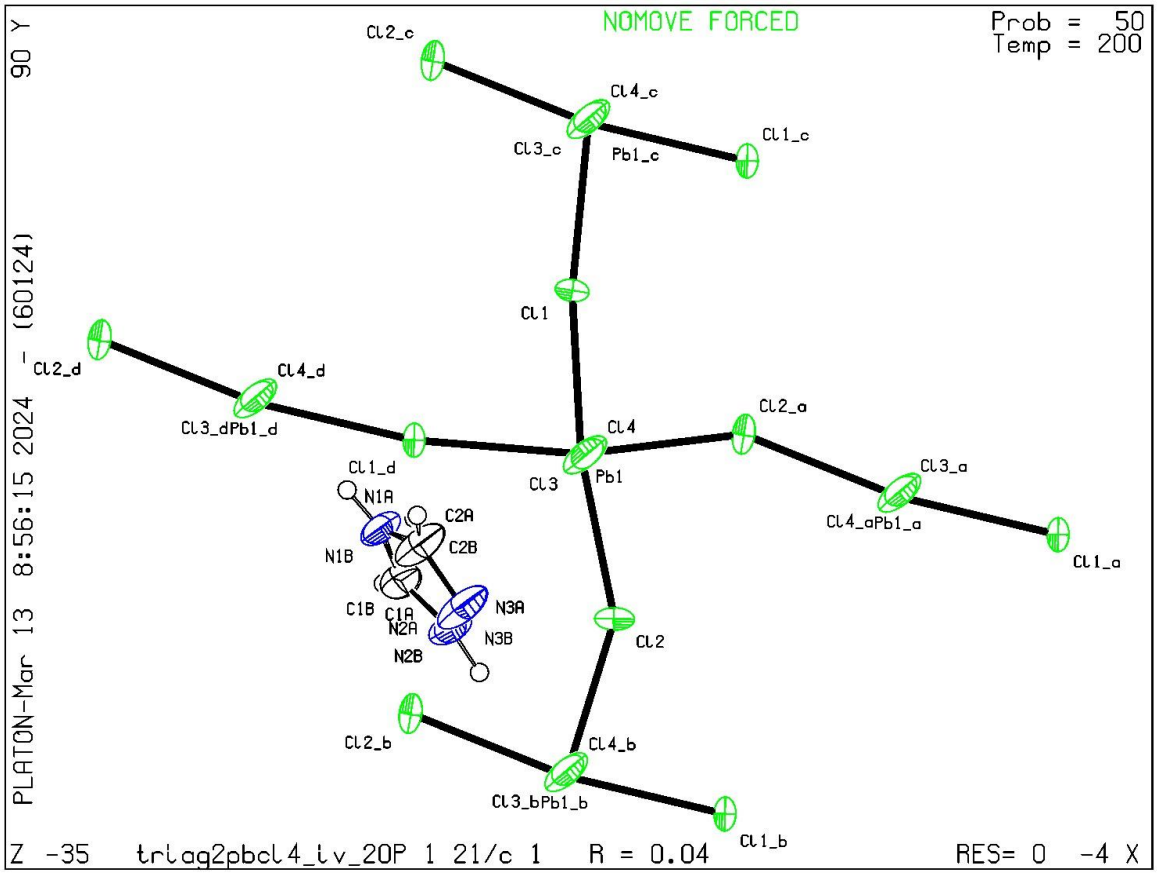

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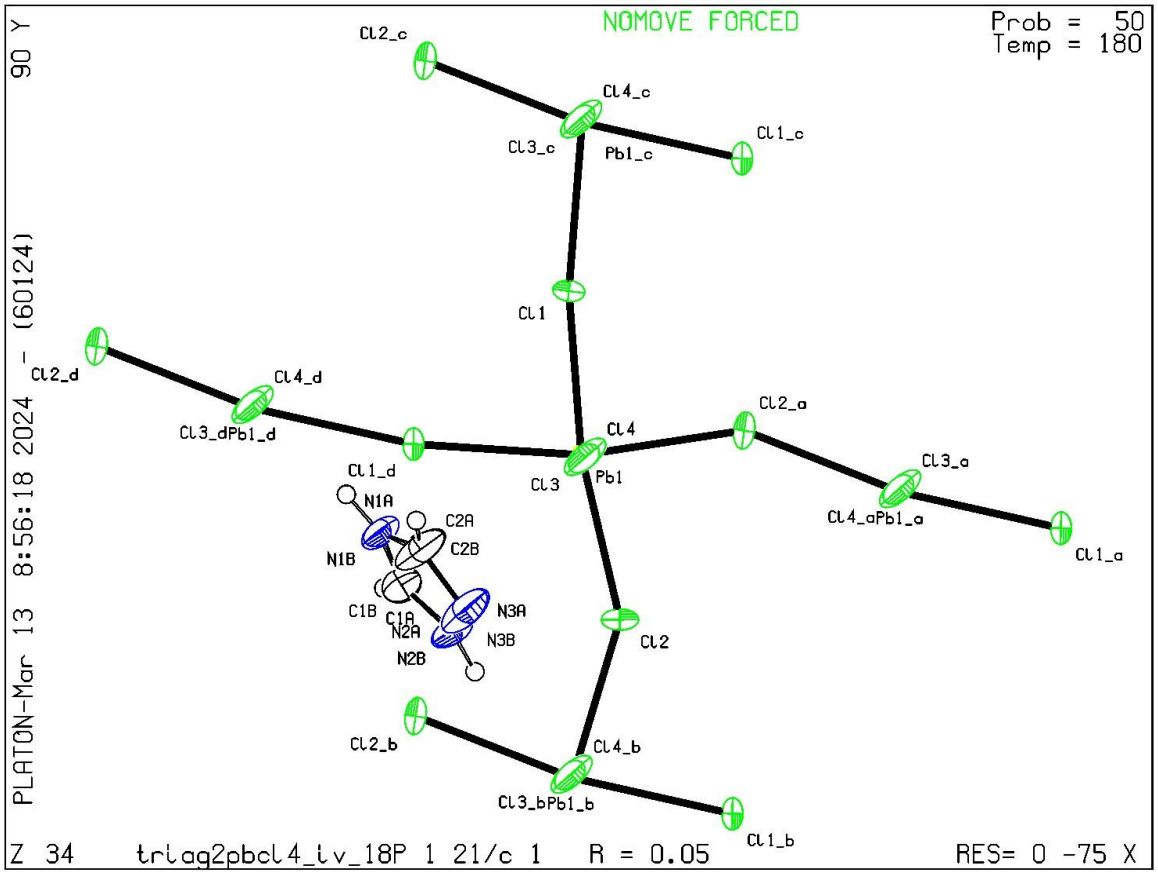

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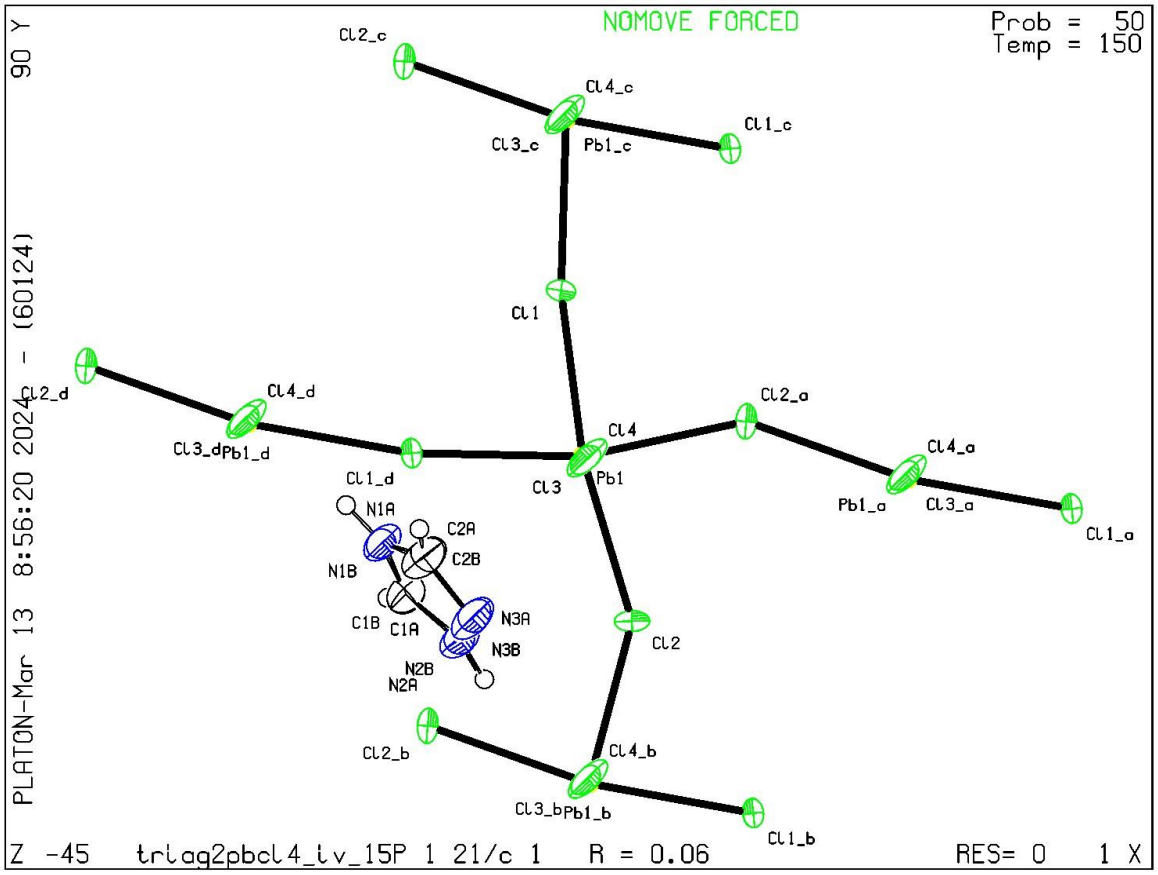

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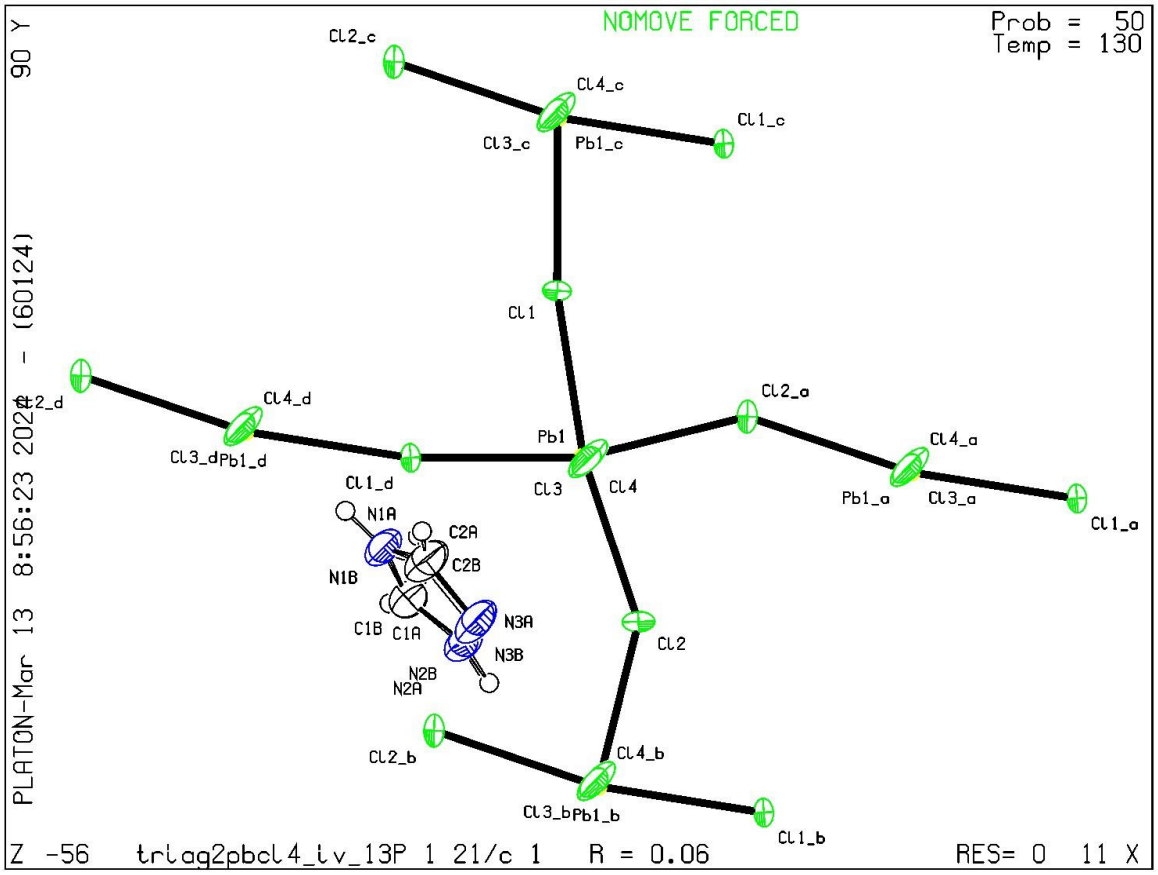

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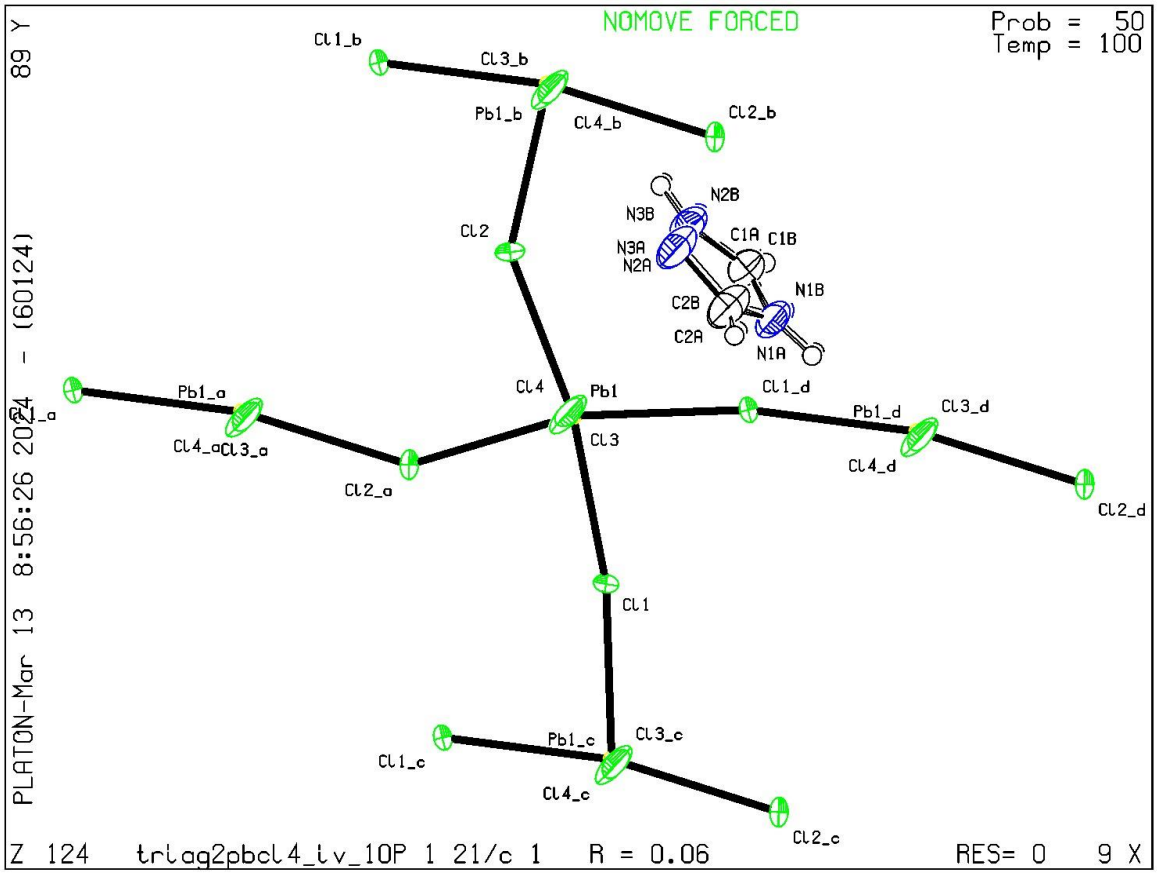
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RES= 0 9 X
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Cl3_b
Pb1_b
Cl4_b
Cl2_b
N2B
N3B
N3A
N2A
C1A
C1B
N1B
C2B
C2A
N1A
Cl2
Cl4
Pb1
Cl1_d
Pb1_d
Cl3_d
Cl4_d
Cl2_d
Pb1_a
Cl4_a
Cl3_a
Cl2_a
Cl3
Cl1
Pb1_c
Cl3_c
Cl1_c
Cl4_c
Cl2_c