Supplementary material for:

***White light emission from a zero-dimensional lead-chloride hybrid material***

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Table S1. Crystallographic data for (TAE)2[Pb2Cl10](Cl)2.

|  |  |
| --- | --- |
| Chemical formula | (C6N4H22)2[Pb2Cl10]Cl2 |
| Chemical formula moiety | Cl10 Pb2, 2(C6 H22 N4), 2(Cl) |
| Formula weight/gmol-1 | 1140.33 |
| Crystalsystem | triclinic |
| Space group | P-1 |
| a/Å | 9.9851(10) |
| b/Å | 10.2719(10) |
| c/Å | 18.4551(17) |
| α/° | 74.596(3) |
| β/° | 85.797(4) |
| γ/° | 67.643(3) |
| Volume/Å3 | 1686.9(3) |
| Z | 2 |
| Temperature (K) | 100(2) |
| Collected reflections | 177910 |
| /° | 2.206-36.418 |
| Crystal colour | colourless |
| F(000) | 1080 |
| Absorption coefficient | 10.938 |
| Radiation source (wavelength) | MoK\a (0.71073) |
| hmin- hmax; kmin-kmax; lmin-lmax/° | -16-16 ; -17-17 ; -30-30 |
| Rint | 0.0556 |
| aR1 [F2> 2\*s(F2)] | 0.0306 [0.0219] |
| awR2 [F2> 2\*s(F2)] | 0.0526 [0.0454] |
| bGoodness-of-fit on F2 | 1.154 |
| Largest diff. peak/hole / e- Å-3 | 1.291 / -1.604 |

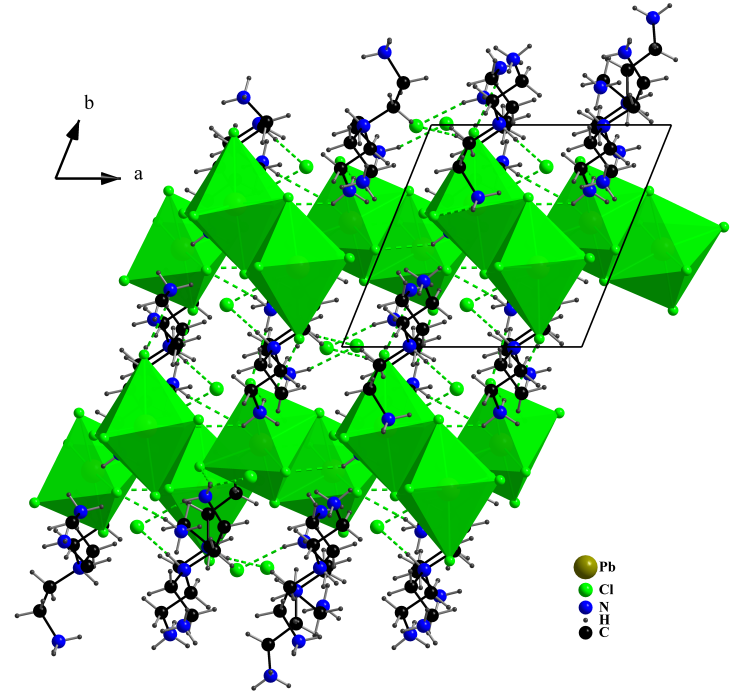
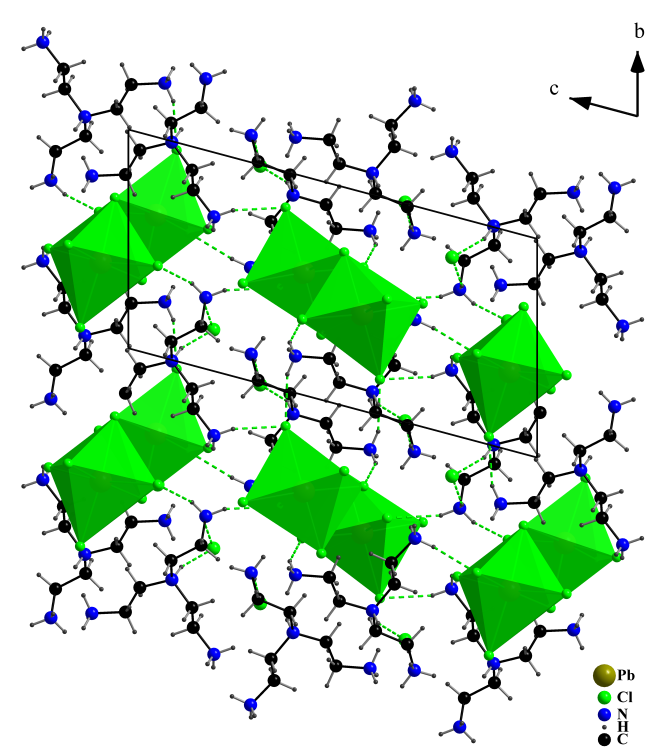
*aR1=Σ(Fo-Fc|/Fo) and wR2= {Σ[w(Fo2-Fc2)2]/ Σ[w(Fo2)2]}1/2*

*bG.O.F = [(Σ(w(Fo2-Fc2))2/(Nobs-Nvar)]1/2*

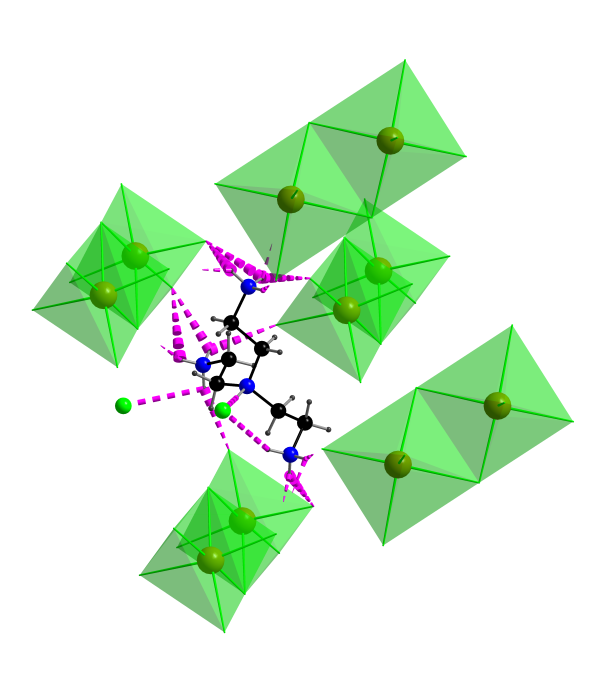
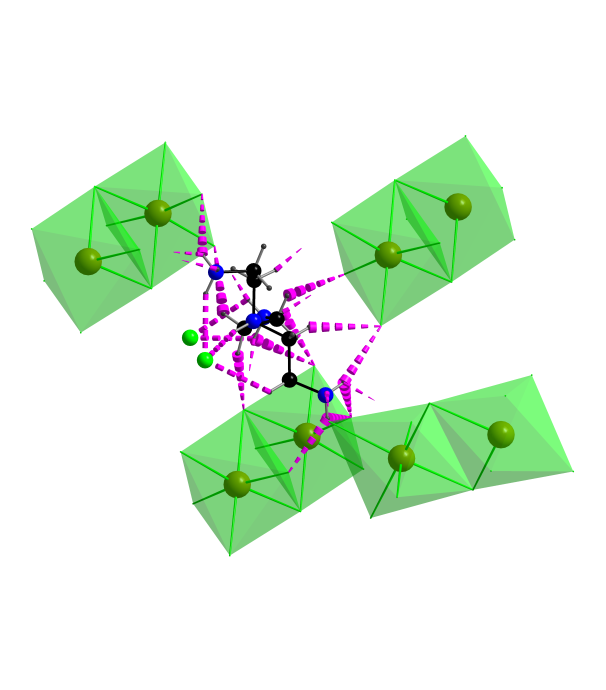
Table S2. Experimental bond lengths and angles of the two [Pb2Cl10]6-groups.

|  |  |  |  |
| --- | --- | --- | --- |
| Bond | Length (Å) | Angle | Value (°) |
| Pb1-Cl4 | 2.7724(5) | Cl4-Pb1-Cl3 | 87.252(16) |
| Pb1-Cl3 | 2.7840(5) | Cl4-Pb1-Cl5 | 83.671(14) |
| Pb1-Cl5 | 2.9078(6) | Cl3-Pb1-Cl5 | 87.174(15) |
| Pb1-Cl1 | 2.9345(5) | Cl4-Pb1-Cl1 | 170.175(14) |
| Pb1-Cl2 | 2.9599(6) | Cl3-Pb1-Cl1 | 91.010(15) |
| Pb1-Cl5 | 3.0488(5) | Cl5-Pb1-Cl1 | 86.587(14) |
| Pb2-Cl7 | 2.7835(5) | Cl4-Pb1-Cl2 | 88.480(15) |
| Pb2-Cl9 | 2.8406(5) | Cl3-Pb1-Cl2 | 95.037(15) |
| Pb2-Cl8 | 2.8624(5) | Cl5-Pb1-Cl2 | 171.740(14) |
| Pb2-Cl10 | 2.9397(6) | Cl1-Pb1-Cl2 | 101.309(15) |
| Pb2-Cl6 | 2.9523(6) | Cl4-Pb1-Cl5 | 97.068(15) |
| Pb2-Cl9 | 3.0430(6) | Cl3-Pb1-Cl5 | 174.998(14) |
|  |  | Cl5-Pb1-Cl5 | 90.787(14) |
|  |  | Cl1-Pb1-Cl5 | 84.306(15) |
|  |  | Cl2-Pb1-Cl5 | 87.622(14) |
|  |  | Cl7-Pb2-Cl9 | 91.798(16) |
|  |  | Cl7-Pb2-Cl8 | 90.723(15) |
|  |  | Cl9-Pb2-Cl8 | 83.934(15) |
|  |  | Cl7-Pb2-Cl10 | 88.353(15) |
|  |  | Cl9-Pb2-Cl10 | 91.501(15) |
|  |  | Cl8-Pb2-Cl10 | 175.313(14) |
|  |  | Cl7-Pb2-Cl6 | 91.297(15) |
|  |  | Cl9-Pb2-Cl6 | 176.750(14) |
|  |  | Cl8-Pb2-Cl6 | 97.021(15) |
|  |  | Cl10-Pb2-Cl6 | 87.595(15) |
|  |  | Cl7-Pb2-Cl9 | 166.464(14) |
|  |  | Cl9-Pb2-Cl9 | 89.539(15) |
|  |  | Cl8-Pb2-Cl9 | 76.021(15) |
|  |  | Cl10-Pb2-Cl9 | 105.081(15) |
|  |  | Cl6-Pb2-Cl9 | 87.684(15) |
|  |  | Pb1-Cl5-Pb1 | 89.213(14) |
|  |  | Pb2-Cl9-Pb2 | 90.461(15) |

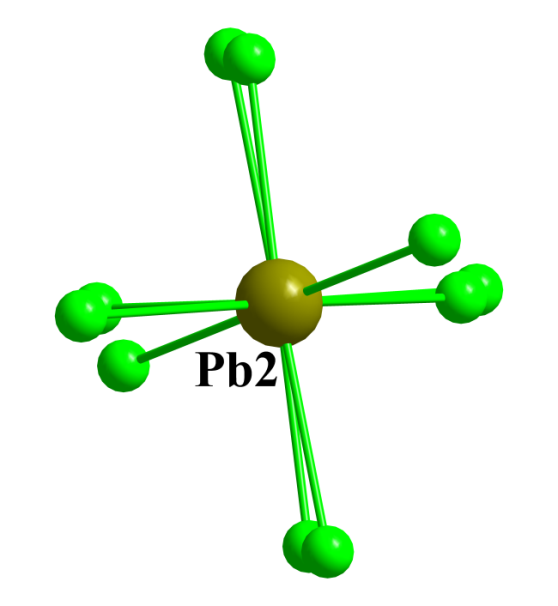
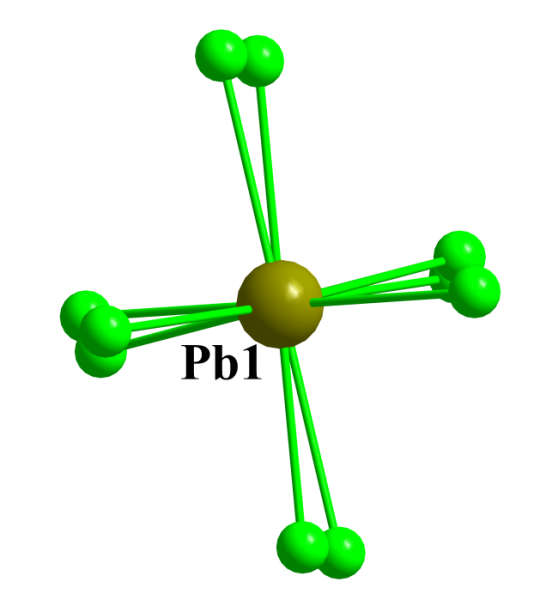
**Figure S1.**Crystal structure of the (TAE)2[Pb2Cl10](Cl)2 projected along the (left) a-axis and (right) c-axis.

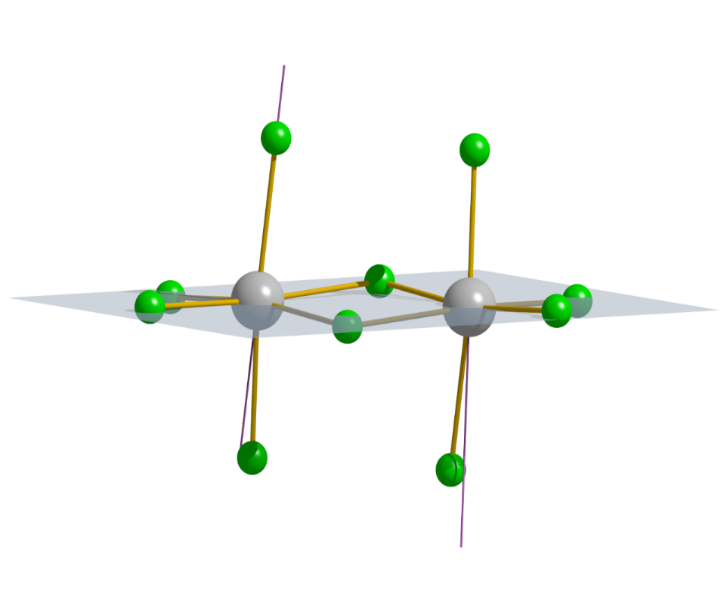


**Figure S2.** N-H…Cl hydrogen bonds in (TAE)2[Pb2Cl10](Cl)2. The two symmetry independent [TAE]4+ cations are involved in a dense network of N-H…Cl hydrogen bonds.(left) The first cation is connected to four **[**Pb2Cl10**]6-** groups and 2 Cl- ions; (right) the second cation is connected to five **[**Pb2Cl10**]6-** groups and 2 Cl- ions.



**Figure S3.** Structural distortion of the two **[**Pb2Cl10**]6-**groups. The geometries of the two **[**Pb2Cl10**]6-** groups is quite different

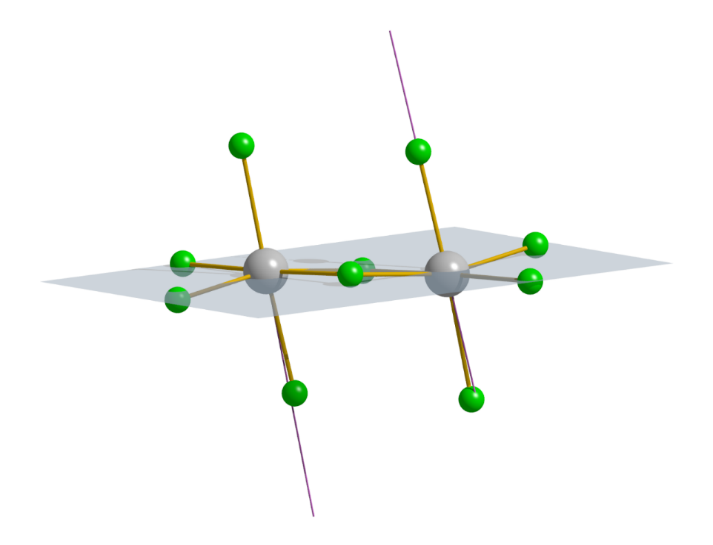




86.03(2)°

Pb1

81.36(2)°

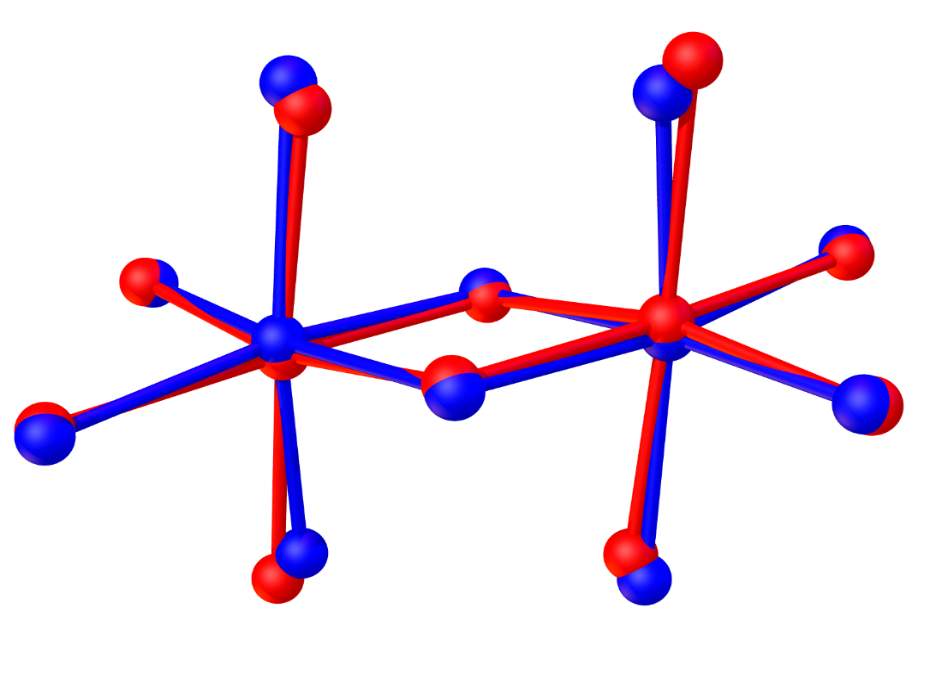


Pb2

78.71(2)°

99.24(2)°

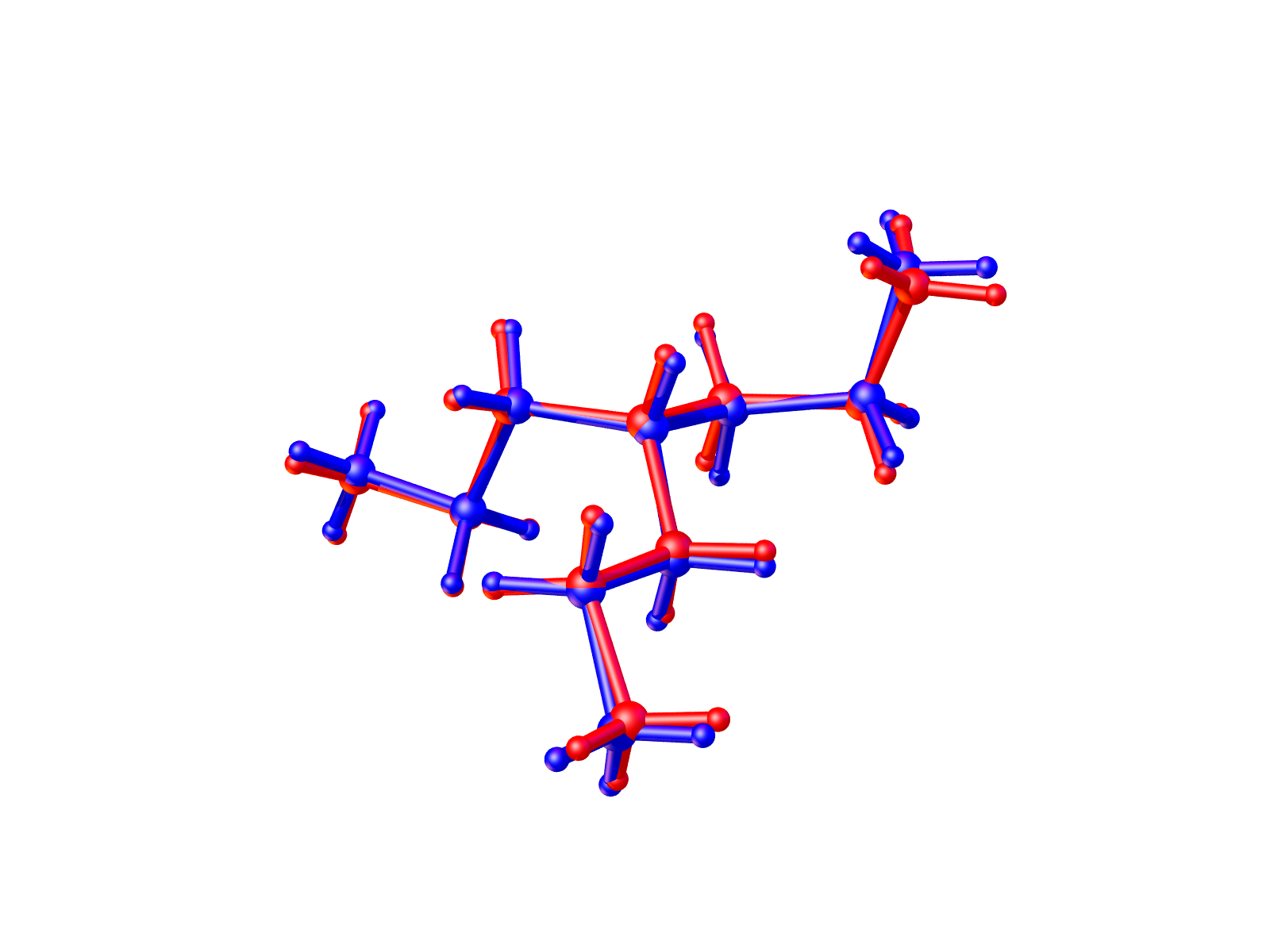
**Figure S4.** Superposition of the two **[**Pb2Cl10**]6-** groups.



**Pb1**

**Pb2**

**Figure S5.** Superposition of the [TAE]4+ cations. The two [TAE]4+ adopt the same conformation



**Figure S6.** Room temperature Raman spectrum of (TAE)2[Pb2Cl10](Cl)2.

