

Crystal structure of (μ_4 -oxygen)tetra(2-(4'-chlorobenzoyl)benzoato)trilead(II), $\text{Pb}_3\text{O}(\text{C}_{14}\text{H}_8\text{O}_3\text{Cl})_4$

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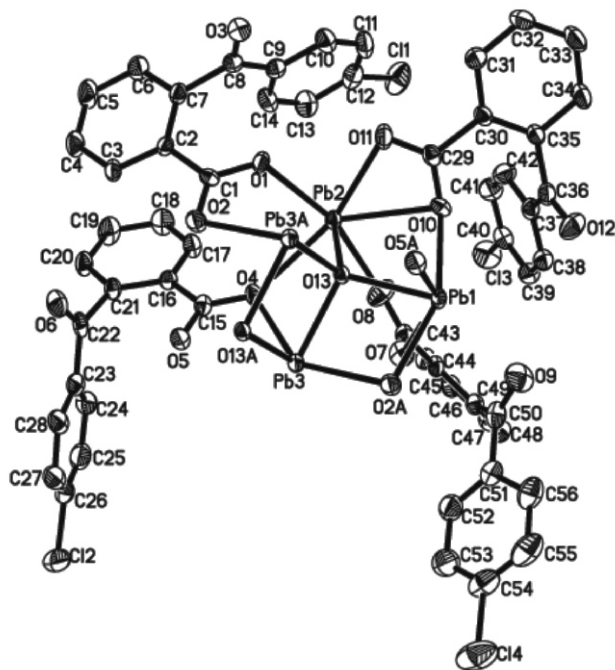


Table 2. Continued.

Atom	Site	x	y	z	<i>U</i> _{iso}
H(13A)	4e	-0.1475	0.1437	0.2652	0.074
H(41A)	4e	-0.3466	-0.1179	0.2467	0.070
H(45A)	4e	-0.5151	-0.0116	0.3779	0.055
H(17A)	4e	-0.1801	0.2174	0.3812	0.057
H(10A)	4e	0.2043	-0.0006	0.2819	0.062
H(3A)	4e	0.1408	0.3060	0.4501	0.049
H(6A)	4e	0.2361	0.2992	0.3035	0.070
H(14A)	4e	0.0011	0.1981	0.3118	0.064
H(46A)	4e	-0.7109	-0.0482	0.3698	0.056
H(31A)	4e	0.1894	-0.1826	0.3098	0.056
H(34A)	4e	-0.0659	-0.4117	0.2857	0.069
H(20A)	4e	-0.1006	0.4883	0.4392	0.061
H(39A)	4e	-0.5394	-0.2312	0.3375	0.065

Table 2. Continued.

Atom	Site	x	y	z	<i>U</i> _{iso}
H(42A)	4e	-0.1838	-0.1943	0.2734	0.065
H(5A)	4e	0.2119	0.4299	0.3394	0.079
H(32A)	4e	0.2401	-0.2954	0.2644	0.069
H(33A)	4e	0.1072	-0.4062	0.2493	0.077
H(19A)	4e	-0.1492	0.4738	0.3653	0.079
H(24A)	4e	-0.2994	0.4206	0.4930	0.067
H(28A)	4e	-0.0591	0.3682	0.5890	0.068
H(52A)	4e	-0.5449	-0.1197	0.5287	0.076
H(27A)	4e	-0.1993	0.3850	0.6407	0.082
H(56A)	4e	-0.4081	-0.3574	0.5333	0.085
H(25A)	4e	-0.4356	0.4471	0.5463	0.088
H(53A)	4e	-0.5827	-0.1294	0.6036	0.089
H(55A)	4e	-0.4564	-0.3692	0.6064	0.102

Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
Pb(1)	4e	-0.11281(2)	-0.18944(1)	0.460215(6)	0.0431(1)	0.0213(1)	0.0286(1)	-0.00572(8)	-0.00200(8)	-0.00039(7)
Pb(2)	4e	-0.08407(2)	0.00734(1)	0.391938(6)	0.0390(1)	0.0249(1)	0.0252(1)	-0.00288(8)	-0.00257(8)	0.00203(7)
Pb(3)	4e	-0.14912(2)	0.02241(1)	0.513641(6)	0.0337(1)	0.0253(1)	0.0303(1)	-0.00242(8)	0.00145(8)	-0.00197(8)
Cl(3)	4e	-0.5791(2)	-0.1107(2)	0.26934(7)	0.072(1)	0.089(2)	0.089(2)	0.019(1)	-0.009(1)	0.008(1)
Cl(1)	4e	-0.1639(2)	-0.0011(2)	0.20913(8)	0.095(2)	0.096(2)	0.076(2)	-0.041(1)	-0.032(1)	0.003(1)
O(3)	4e	0.3101(4)	0.1030(3)	0.3326(1)	0.052(2)	0.048(3)	0.050(3)	-0.001(2)	0.003(2)	-0.002(2)
C(2)	4e	0.1665(4)	0.2253(3)	0.3995(2)	0.034(3)	0.026(3)	0.033(3)	-0.005(2)	0.001(2)	0.002(2)
O(13)	4e	-0.0424(3)	-0.0486(2)	0.4598(1)	0.037(2)	0.023(2)	0.023(2)	-0.003(1)	-0.002(1)	-0.001(1)
C(44)	4e	-0.4693(5)	-0.1027(4)	0.4226(2)	0.040(3)	0.032(3)	0.045(3)	-0.005(2)	-0.002(2)	-0.008(3)
C(16)	4e	-0.1362(4)	0.2800(3)	0.4379(2)	0.036(3)	0.028(3)	0.034(3)	0.002(2)	-0.001(2)	0.004(2)
O(1)	4e	0.1206(3)	0.0756(2)	0.4014(1)	0.052(2)	0.031(2)	0.035(2)	-0.016(2)	0.004(2)	-0.000(2)
C(30)	4e	0.0312(5)	-0.2303(3)	0.3257(2)	0.048(3)	0.031(3)	0.027(3)	0.003(2)	0.002(2)	-0.003(2)
C(9)	4e	0.1178(5)	0.1055(4)	0.3010(2)	0.053(3)	0.035(3)	0.028(3)	-0.004(3)	0.004(2)	0.009(2)
C(21)	4e	-0.1124(4)	0.3623(4)	0.4549(2)	0.045(3)	0.023(3)	0.044(3)	0.002(2)	-0.002(3)	0.001(2)
O(4)	4e	-0.1491(4)	0.1274(2)	0.4486(1)	0.067(2)	0.022(2)	0.038(2)	0.005(2)	0.001(2)	0.000(2)
C(38)	4e	-0.3707(6)	-0.2684(4)	0.3408(2)	0.068(4)	0.044(4)	0.044(4)	-0.009(3)	0.008(3)	-0.004(3)
C(1)	4e	0.1410(4)	0.1439(3)	0.4232(2)	0.035(3)	0.036(3)	0.023(3)	0.004(2)	0.001(2)	-0.002(2)
C(4)	4e	0.1725(6)	0.3809(4)	0.3976(2)	0.078(5)	0.024(3)	0.061(4)	-0.005(3)	0.004(3)	-0.001(3)
O(10)	4e	-0.0918(3)	-0.1611(3)	0.3767(1)	0.055(2)	0.046(2)	0.033(2)	-0.005(2)	0.011(2)	-0.014(2)
C(29)	4e	0.0008(5)	-0.1548(4)	0.3551(2)	0.045(3)	0.032(3)	0.030(3)	0.004(3)	-0.004(2)	-0.002(2)
C(47)	4e	-0.7024(5)	-0.1482(4)	0.4126(2)	0.038(3)	0.052(4)	0.044(4)	-0.005(3)	-0.004(3)	-0.016(3)
C(48)	4e	-0.6308(5)	-0.1937(4)	0.4421(2)	0.045(3)	0.040(4)	0.053(4)	-0.002(3)	0.002(3)	0.008(3)
C(40)	4e	-0.4572(5)	-0.1678(4)	0.2894(2)	0.057(4)	0.044(4)	0.053(4)	0.004(3)	-0.002(3)	-0.010(3)
C(36)	4e	-0.1609(5)	-0.3063(4)	0.3406(2)	0.060(4)	0.030(3)	0.040(3)	-0.006(3)	0.002(3)	-0.004(3)
C(43)	4e	-0.3438(5)	-0.0756(4)	0.4281(2)	0.038(3)	0.037(3)	0.051(4)	-0.002(3)	-0.001(3)	-0.008(3)
C(18)	4e	-0.1691(6)	0.3437(5)	0.3657(2)	0.094(5)	0.058(5)	0.039(4)	-0.007(4)	-0.014(3)	0.009(3)
C(11)	4e	0.0476(7)	-0.0047(4)	0.2502(2)	0.093(6)	0.037(4)	0.053(4)	-0.013(4)	-0.004(4)	-0.009(3)
O(2)	4e	0.1335(4)	0.1433(2)	0.4645(1)	0.075(3)	0.035(2)	0.028(2)	-0.004(2)	0.008(2)	0.002(2)
O(5)	4e	-0.1023(3)	0.2086(2)	0.5066(1)	0.054(2)	0.033(2)	0.032(2)	0.002(2)	-0.003(2)	0.002(2)
O(11)	4e	0.0639(3)	-0.0902(3)	0.3570(2)	0.045(2)	0.032(2)	0.076(3)	-0.007(2)	0.004(2)	-0.013(2)
C(13)	4e	-0.0763(6)	0.1149(5)	0.2685(2)	0.064(4)	0.054(5)	0.067(5)	0.005(4)	-0.009(4)	0.000(4)
O(7)	4e	-0.2879(3)	-0.0975(3)	0.4625(2)	0.041(2)	0.066(3)	0.064(3)	-0.001(2)	-0.010(2)	-0.005(2)
O(12)	4e	-0.1687(4)	-0.3558(3)	0.3711(2)	0.065(3)	0.054(3)	0.075(3)	-0.003(2)	0.008(2)	0.024(3)
C(41)	4e	-0.3527(6)	-0.1559(5)	0.2703(2)	0.070(4)	0.060(5)	0.044(4)	0.003(4)	0.000(3)	0.008(3)
O(8)	4e	-0.3003(4)	-0.0310(3)	0.3983(2)	0.042(2)	0.078(4)	0.088(4)	-0.013(2)	-0.002(2)	0.021(3)
C(45)	4e	-0.5441(5)	-0.0576(4)	0.3940(2)	0.046(3)	0.038(3)	0.054(4)	-0.002(3)	0.002(3)	0.003(3)
C(15)	4e	-0.1281(4)	0.2004(3)	0.4656(2)	0.025(2)	0.025(3)	0.048(3)	0.005(2)	-0.003(2)	-0.001(2)
C(37)	4e	-0.2628(5)	-0.2573(4)	0.3219(2)	0.051(3)	0.034(3)	0.038(3)	-0.007(3)	-0.002(3)	-0.005(2)
C(49)	4e	-0.5128(5)	-0.1716(4)	0.4475(2)	0.036(3)	0.036(3)	0.043(3)	-0.001(2)	-0.003(2)	-0.005(3)
C(8)	4e	0.2152(5)	0.1384(4)	0.3306(2)	0.055(3)	0.035(3)	0.025(3)	-0.005(3)	0.007(2)	0.005(2)
C(17)	4e	-0.1643(5)	0.2720(4)	0.3930(2)	0.066(4)	0.035(3)	0.040(3)	-0.004(3)	-0.009(3)	-0.002(3)
C(10)	4e	0.1337(6)	0.0289(4)	0.2782(2)	0.070(4)	0.042(4)	0.042(4)	0.002(3)	-0.001(3)	-0.004(3)
C(35)	4e	-0.0459(5)	-0.2981(4)	0.3186(2)	0.054(3)	0.030(3)	0.036(3)	0.000(3)	0.008(3)	-0.005(2)
C(3)	4e	0.1573(5)	0.3042(3)	0.4204(2)	0.053(3)	0.028(3)	0.041(3)	-0.009(3)	0.002(3)	-0.004(2)
C(7)	4e	0.1965(5)	0.2221(4)	0.3550(2)	0.051(3)	0.030(3)	0.033(3)	-0.010(3)	0.000(2)	0.003(2)
C(6)	4e	0.2148(6)	0.2999(4)	0.3328(2)	0.093(5)	0.045(4)	0.037(4)	-0.018(4)	0.008(3)	0.005(3)
C(14)	4e	0.0130(6)	0.1472(4)	0.2962(2)	0.077(5)	0.040(4)	0.043(4)	0.003(3)	0.001(3)	-0.007(3)
C(46)	4e	-0.6612(5)	-0.0794(4)	0.3889(2)	0.046(3)	0.039(4)	0.054(4)	0.009(3)	-0.005(3)	-0.001(3)
C(12)	4e	-0.0561(6)	0.0393(5)	0.2461(2)	0.075(5)	0.054(4)	0.039(4)	-0.022(4)	-0.009(3)	0.007(3)
C(31)	4e	0.1383(5)	-0.2288(4)	0.3050(2)	0.060(4)	0.041(4)	0.039(3)	-0.003(3)	0.009(3)	0.004(3)

Table 3. Continued.

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(34)	4e	−0.0154(6)	−0.3650(4)	0.2904(2)	0.083(5)	0.037(4)	0.054(4)	−0.004(3)	0.009(4)	−0.016(3)
C(20)	4e	−0.1170(6)	0.4336(4)	0.4276(2)	0.079(4)	0.026(3)	0.048(4)	−0.008(3)	−0.003(3)	0.003(3)
C(39)	4e	−0.4677(6)	−0.2238(4)	0.3248(2)	0.054(4)	0.054(4)	0.054(4)	−0.007(3)	0.009(3)	−0.008(3)
C(42)	4e	−0.2551(6)	−0.2015(4)	0.2866(2)	0.056(4)	0.061(4)	0.048(4)	−0.010(3)	0.008(3)	0.002(3)
C(5)	4e	0.2012(7)	0.3782(4)	0.3545(2)	0.112(6)	0.029(4)	0.058(5)	−0.014(4)	0.002(4)	0.010(3)
C(32)	4e	0.1680(6)	−0.2954(4)	0.2774(2)	0.068(4)	0.056(4)	0.050(4)	0.006(3)	0.025(3)	−0.005(3)
C(33)	4e	0.0894(7)	−0.3626(5)	0.2691(2)	0.093(5)	0.049(4)	0.052(4)	0.005(4)	0.015(4)	−0.021(3)
C(19)	4e	−0.1456(7)	0.4251(4)	0.3833(2)	0.100(6)	0.038(4)	0.058(5)	−0.003(4)	−0.011(4)	0.021(3)
O(6)	4e	0.0292(4)	0.3784(3)	0.5134(2)	0.054(3)	0.054(3)	0.059(3)	−0.003(2)	−0.012(2)	−0.016(2)
O(9)	4e	−0.3630(4)	−0.2748(3)	0.4615(2)	0.083(3)	0.063(3)	0.083(4)	0.030(3)	0.007(3)	0.006(3)
C(22)	4e	−0.0744(6)	0.3765(3)	0.5029(2)	0.064(4)	0.018(3)	0.046(4)	0.000(3)	−0.008(3)	−0.003(2)
C(23)	4e	−0.1662(5)	0.3912(3)	0.5357(2)	0.061(4)	0.019(3)	0.051(4)	0.001(3)	0.004(3)	0.005(2)
C(50)	4e	−0.4411(5)	−0.2303(4)	0.4767(2)	0.050(4)	0.036(4)	0.071(5)	0.000(3)	−0.008(3)	0.002(3)
C(24)	4e	−0.2785(6)	0.4148(4)	0.5228(2)	0.066(4)	0.043(4)	0.057(4)	−0.003(3)	0.008(3)	−0.001(3)
C(51)	4e	−0.4704(5)	−0.2365(4)	0.5240(2)	0.045(3)	0.047(4)	0.053(4)	−0.004(3)	−0.009(3)	0.008(3)
C(28)	4e	−0.1355(7)	0.3822(4)	0.5802(2)	0.098(5)	0.026(3)	0.046(4)	−0.001(3)	0.010(4)	0.004(3)
C(52)	4e	−0.5242(6)	−0.1694(5)	0.5445(2)	0.075(5)	0.055(4)	0.061(5)	−0.006(4)	−0.001(4)	0.003(4)
C(26)	4e	−0.3271(8)	0.4182(4)	0.5979(3)	0.108(6)	0.030(4)	0.075(6)	−0.021(4)	0.043(5)	−0.007(4)
C(27)	4e	−0.2182(8)	0.3938(4)	0.6110(2)	0.126(7)	0.034(4)	0.048(4)	−0.007(4)	0.020(4)	0.004(3)
C(56)	4e	−0.4442(7)	−0.3114(5)	0.5471(3)	0.075(5)	0.056(5)	0.081(6)	−0.003(4)	−0.018(4)	0.021(4)
C(54)	4e	−0.5202(7)	−0.2505(7)	0.6113(3)	0.069(5)	0.101(7)	0.054(5)	−0.028(5)	−0.014(4)	0.018(5)
C(25)	4e	−0.3600(7)	0.4297(5)	0.5544(3)	0.067(5)	0.050(5)	0.106(7)	−0.012(4)	0.021(4)	−0.015(5)
C(53)	4e	−0.5483(6)	−0.1754(6)	0.5892(3)	0.074(5)	0.081(6)	0.067(5)	−0.010(4)	0.000(4)	−0.002(4)
C(55)	4e	−0.4716(7)	−0.3180(6)	0.5910(3)	0.089(6)	0.082(7)	0.082(6)	−0.008(5)	−0.018(5)	0.046(5)
Cl(2)	4e	−0.4314(3)	0.4384(2)	0.63715(9)	0.162(2)	0.079(2)	0.132(2)	−0.036(2)	0.099(2)	−0.027(2)
Cl(4)	4e	−0.5483(2)	−0.2572(2)	0.66757(7)	0.117(2)	0.179(3)	0.060(1)	−0.049(2)	−0.011(1)	0.028(2)

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