Table 1. Crystal data for $(Bert*Pb)_2$ + hexane.

Identification code	bt73
Empirical formula	$C_{78}H_{112}Pb_2$
Formula weight	1464.06
Crystal size	0.26 x 0.24 x 0.15 mm
Crystal habit	block
Crystal color	green/brown
Crystal system	Monoclinic
Space group	P2(1)/c
Unit cell dimensions	a = 13.3312(3) Å α = 90° b = 15.9539(4) Å β = 103.7200(10)° c = 16.8793(4) Å γ = 90°
Volume	3487.53(14) $Å^3$
Z	2
Density (calculated)	1.394 $Mg \cdot m^{-3}$
Absorption coefficient	4.861 mm^{-1}
F(000)	1488
Absorption correction[1]	Empirical
Max. and min. transmission	0.448108 and 0.326622

1) SADABS: an empirical absorption correction program by G.M. Sheldrick; using the method described by Blessing, R.H. *Acta Cryst.* 1995 ,A51, 33.

Table 2. Data collection for $(Bert*Pb)_2$ + hexane.

Diffractometer	Bruker SMART 1000
Temperature	93(2) K
Radiation source	normal-focus sealed tube
Wavelength	0.71073 Å (MoKα)
Monochromator	graphite
θ range for data collection	1.78 to 31.50°
Scan type	ω
Index ranges	$-19 \le h \le 18$, $0 \le k \le 23$, $0 \le l \le 24$
Reflections collected	28976
Independent reflections	11316 (R_{int} = 0.0348)
Standard reflections	50 frames remeasured
Percent decay of standards	<0.01

Table 3. Solution and refinement of $(Bert*Pb)_2$ + hexane.

System for solution	XS, Bruker SHELXTL v. 5.10
Structure solution	direct
System for refinement	XL, Bruker SHELXTL v. 5.10
Refinement method	Full-matrix least-squares on F^2
Hydrogen atoms	constr
Data / restraints / parameters	11316 / 0 / 362
Goodness-of-fit on F^2	0.939
Weighting scheme	$w^{-1} = \sigma^2(Fo^2) + (0.0407P)^2 + 0.00P$, where $P = (Fo^2 + 2Fc^2)/3$
R indices (all data)	R1 = 0.0269, wR2 = 0.0553
R indices calcd from obsd data	R1 = 0.0206, wR2 = 0.0536
Observed data (>2sigma(I))	9721
Extinction coefficient	0.00000(6)
Largest diff. peak and hole	1.414 and -0.546 eÅ^{-3}

1) $R1 = \sum||Fo-Fc||/\sum|Fo|$

$wR2 = [\sum[w(Fo^2-Fc^2)^2]/\sum[w(Fo^2)^2]]^{½}$

2) Goodness-of-Fit = $[\sum[w(Fo^2-Fc^2)^2]/(M-N)]^{½}$

where M is the number of reflections
and N is the number of parameters refined.

3) Refinement is based on F^2 for ALL reflections except for those with very negative F^2 or flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The observed criterion of $F^2 > 2\sigma(F^2)$ is used only for calculating R indices for observed data and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

Table 4. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for $(Bert*Pb)_2$ + hexane.
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pb(1)	4126(1)	5351(1)	4260(1)	16(1)
C(1)	2786(1)	4971(1)	4831(1)	11(1)
C(2)	2444(1)	5619(1)	5271(1)	11(1)
C(3)	1637(1)	5487(1)	5652(1)	14(1)
C(4)	1151(1)	4710(1)	5599(1)	14(1)
C(5)	1453(1)	4076(1)	5138(1)	13(1)
C(6)	2253(1)	4203(1)	4746(1)	11(1)
C(7)	2454(1)	3528(1)	4183(1)	11(1)
C(8)	3031(1)	2805(1)	4480(1)	12(1)
C(9)	3114(1)	2163(1)	3935(1)	14(1)
C(10)	2635(1)	2209(1)	3108(1)	13(1)
C(11)	2078(1)	2930(1)	2827(1)	13(1)
C(12)	1975(1)	3590(1)	3346(1)	13(1)
C(13)	2896(1)	6484(1)	5294(1)	12(1)
C(14)	3661(1)	6757(1)	5978(1)	13(1)
C(15)	3963(1)	7596(1)	6028(1)	14(1)
C(16)	3538(1)	8175(1)	5421(1)	14(1)
C(17)	2817(1)	7890(1)	4740(1)	14(1)
C(18)	2489(1)	7055(1)	4660(1)	13(1)
C(19)	1663(1)	6790(1)	3912(1)	18(1)
C(20)	596(2)	7090(1)	3996(1)	27(1)
C(21)	1882(2)	7099(1)	3113(1)	25(1)
C(22)	3896(1)	9082(1)	5531(1)	16(1)
C(23)	3523(2)	9494(1)	6229(1)	24(1)
C(24)	3578(2)	9620(1)	4762(1)	23(1)
C(25)	4133(1)	6157(1)	6664(1)	15(1)
C(26)	5305(1)	6257(1)	6946(1)	23(1)
C(27)	3629(2)	6267(1)	7387(1)	24(1)
C(28)	3509(1)	2701(1)	5389(1)	14(1)
C(29)	2888(2)	2068(1)	5766(1)	20(1)
C(30)	4644(1)	2439(1)	5570(1)	21(1)
C(31)	2643(1)	1482(1)	2523(1)	15(1)
C(32)	2028(2)	743(1)	2740(1)	21(1)
C(33)	3731(2)	1208(1)	2487(1)	21(1)
C(34)	1284(1)	4327(1)	2994(1)	17(1)
C(35)	1639(2)	4754(1)	2296(1)	26(1)
C(36)	153(2)	4044(1)	2722(1)	28(1)
C(40)	-253(2)	8242(2)	5852(2)	38(1)
C(41)	-536(2)	9144(2)	5621(1)	31(1)
C(42)	127(2)	9542(1)	5101(1)	28(1)

Table 5. Bond lengths [Å] for $(Bert*Pb)_2$ + hexane.

Pb(1)-C(1)	2.3032(16)	Pb(1)-Pb(1)#1	3.18811(13)
C(1)-C(6)	1.406(2)	C(1)-C(2)	1.411(2)
C(2)-C(3)	1.395(2)	C(2)-C(13)	1.504(2)
C(3)-C(4)	1.392(2)	C(4)-C(5)	1.393(2)
C(5)-C(6)	1.397(2)	C(6)-C(7)	1.504(2)
C(7)-C(8)	1.410(2)	C(7)-C(12)	1.409(2)
C(8)-C(9)	1.399(2)	C(8)-C(28)	1.524(2)
C(9)-C(10)	1.393(2)	C(10)-C(11)	1.389(2)
C(10)-C(31)	1.524(2)	C(11)-C(12)	1.398(2)
C(12)-C(34)	1.523(2)	C(13)-C(18)	1.411(2)
C(13)-C(14)	1.415(2)	C(14)-C(15)	1.394(2)
C(14)-C(25)	1.518(2)	C(15)-C(16)	1.396(2)
C(16)-C(17)	1.388(2)	C(16)-C(22)	1.521(2)
C(17)-C(18)	1.400(2)	C(18)-C(19)	1.526(2)
C(19)-C(21)	1.528(3)	C(19)-C(20)	1.540(3)
C(22)-C(24)	1.531(3)	C(22)-C(23)	1.531(3)
C(25)-C(26)	1.530(2)	C(25)-C(27)	1.536(3)
C(28)-C(30)	1.530(2)	C(28)-C(29)	1.537(3)
C(31)-C(33)	1.530(2)	C(31)-C(32)	1.529(2)
C(34)-C(35)	1.529(3)	C(34)-C(36)	1.536(3)
C(40)-C(41)	1.514(4)	C(41)-C(42)	1.525(3)
C(42)-C(42)#2	1.521(4)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 #2 -x,-y+2,-z+1

Table 6. Bond angles [°] for $(Bert*Pb)_2$ + hexane.

C(1)-Pb(1)-Pb(1)#1	94.26(4)	C(6)-C(1)-C(2)	118.17(15)		
C(6)-C(1)-Pb(1)	127.69(12)	C(2)-C(1)-Pb(1)	114.02(11)		
C(3)-C(2)-C(1)	120.94(15)	C(3)-C(2)-C(13)	118.28(14)		
C(1)-C(2)-C(13)	120.66(14)	C(2)-C(3)-C(4)	120.21(15)		
C(3)-C(4)-C(5)	119.40(16)	C(4)-C(5)-C(6)	120.84(15)		
C(5)-C(6)-C(1)	120.29(15)	C(5)-C(6)-C(7)	117.78(14)		
C(1)-C(6)-C(7)	121.72(15)	C(8)-C(7)-C(12)	119.62(15)		
C(8)-C(7)-C(6)	121.64(14)	C(12)-C(7)-C(6)	118.49(14)		
C(9)-C(8)-C(7)	119.05(15)	C(9)-C(8)-C(28)	120.19(14)		
C(7)-C(8)-C(28)	120.67(14)	C(10)-C(9)-C(8)	122.15(15)		
C(11)-C(10)-C(9)	117.81(15)	C(11)-C(10)-C(31)	119.58(15)		
C(9)-C(10)-C(31)	122.48(15)	C(12)-C(11)-C(10)	122.28(15)		
C(11)-C(12)-C(7)	119.08(15)	C(11)-C(12)-C(34)	118.55(15)		
C(7)-C(12)-C(34)	122.23(15)	C(18)-C(13)-C(14)	119.58(15)		
C(18)-C(13)-C(2)	119.52(14)	C(14)-C(13)-C(2)	120.67(14)		
C(15)-C(14)-C(13)	119.01(15)	C(15)-C(14)-C(25)	119.88(14)		
C(13)-C(14)-C(25)	121.09(14)	C(14)-C(15)-C(16)	122.06(15)		
C(17)-C(16)-C(15)	118.14(15)	C(17)-C(16)-C(22)	123.24(15)		
C(15)-C(16)-C(22)	118.61(15)	C(16)-C(17)-C(18)	122.00(15)		
C(17)-C(18)-C(13)	119.11(15)	C(17)-C(18)-C(19)	119.39(15)		
C(13)-C(18)-C(19)	121.44(15)	C(18)-C(19)-C(21)	112.96(15)		
C(18)-C(19)-C(20)	109.77(15)	C(21)-C(19)-C(20)	110.80(16)		
C(16)-C(22)-C(24)	114.45(15)	C(16)-C(22)-C(23)	110.65(15)		
C(24)-C(22)-C(23)	109.66(15)	C(14)-C(25)-C(26)	112.30(14)		
C(14)-C(25)-C(27)	110.73(15)	C(26)-C(25)-C(27)	110.30(15)		
C(8)-C(28)-C(30)	112.88(14)	C(8)-C(28)-C(29)	110.54(14)		
C(30)-C(28)-C(29)	109.97(15)	C(10)-C(31)-C(33)	113.26(14)		
C(10)-C(31)-C(32)	110.21(14)	C(33)-C(31)-C(32)	110.91(15)		
C(12)-C(34)-C(35)	112.01(15)	C(12)-C(34)-C(36)	110.47(15)		
C(35)-C(34)-C(36)	111.15(16)	C(40)-C(41)-C(42)	113.7(2)		
C(42)#2-C(42)-C(41)	113.6(2)				

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 #2 -x,-y+2,-z+1

Table 7. Anisotropic displacement parameters [$Å^2 \times 10^3$] for $(Bert*Pb)_2$ + hexane.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^*b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Pb(1)	13(1)	20(1)	17(1)	2(1)	6(1)	-1(1)
C(1)	10(1)	10(1)	13(1)	1(1)	3(1)	-1(1)
C(2)	12(1)	11(1)	11(1)	0(1)	2(1)	-1(1)
C(3)	14(1)	14(1)	14(1)	-3(1)	5(1)	1(1)
C(4)	13(1)	16(1)	15(1)	1(1)	6(1)	-1(1)
C(5)	14(1)	11(1)	14(1)	0(1)	4(1)	-2(1)
C(6)	12(1)	10(1)	11(1)	0(1)	2(1)	1(1)
C(7)	12(1)	10(1)	12(1)	-1(1)	3(1)	-1(1)
C(8)	14(1)	12(1)	11(1)	0(1)	3(1)	0(1)
C(9)	17(1)	11(1)	13(1)	-1(1)	3(1)	2(1)
C(10)	15(1)	12(1)	13(1)	-2(1)	4(1)	-1(1)
C(11)	15(1)	14(1)	11(1)	0(1)	3(1)	0(1)
C(12)	14(1)	12(1)	12(1)	0(1)	3(1)	0(1)
C(13)	12(1)	11(1)	13(1)	-1(1)	4(1)	-1(1)
C(14)	14(1)	11(1)	12(1)	1(1)	4(1)	-1(1)
C(15)	15(1)	13(1)	13(1)	-1(1)	2(1)	-2(1)
C(16)	15(1)	10(1)	16(1)	-1(1)	5(1)	-1(1)
C(17)	16(1)	11(1)	15(1)	2(1)	2(1)	1(1)
C(18)	13(1)	12(1)	14(1)	0(1)	3(1)	0(1)
C(19)	19(1)	14(1)	16(1)	1(1)	-3(1)	-2(1)
C(20)	16(1)	28(1)	33(1)	4(1)	-1(1)	-4(1)
C(21)	30(1)	28(1)	16(1)	0(1)	1(1)	-2(1)
C(22)	18(1)	11(1)	19(1)	0(1)	3(1)	-2(1)
C(23)	33(1)	16(1)	24(1)	-5(1)	7(1)	1(1)
C(24)	31(1)	13(1)	25(1)	2(1)	4(1)	-2(1)
C(25)	18(1)	12(1)	13(1)	2(1)	2(1)	-2(1)
C(26)	19(1)	21(1)	25(1)	8(1)	-3(1)	-2(1)
C(27)	34(1)	23(1)	16(1)	1(1)	8(1)	-3(1)
C(28)	17(1)	14(1)	11(1)	-2(1)	1(1)	3(1)
C(29)	23(1)	22(1)	15(1)	3(1)	5(1)	1(1)
C(30)	19(1)	25(1)	17(1)	-1(1)	1(1)	5(1)
C(31)	20(1)	12(1)	12(1)	-2(1)	3(1)	0(1)
C(32)	29(1)	17(1)	19(1)	-4(1)	7(1)	-5(1)
C(33)	24(1)	19(1)	21(1)	-7(1)	7(1)	2(1)
C(34)	20(1)	14(1)	15(1)	0(1)	1(1)	4(1)
C(35)	29(1)	22(1)	25(1)	11(1)	4(1)	3(1)
C(36)	17(1)	28(1)	37(1)	4(1)	4(1)	8(1)
C(40)	39(1)	41(1)	34(1)	-1(1)	9(1)	-9(1)
C(41)	29(1)	37(1)	28(1)	-7(1)	9(1)	-10(1)
C(42)	23(1)	38(1)	22(1)	-6(1)	6(1)	-4(1)

Table 8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $(Bert*Pb)_2$ + hexane.

	x	y	z	U(eq)
H(3A)	1418	5929	5948	16
H(4A)	618	4613	5875	17
H(5A)	1110	3549	5090	16
H(9A)	3510	1680	4135	17
H(11A)	1757	2975	2262	16
H(15A)	4473	7779	6488	17
H(17A)	2538	8275	4315	17
H(19A)	1650	6163	3895	21
H(20A)	67	6915	3516	40
H(20B)	596	7703	4039	40
H(20C)	445	6844	4487	40
H(21A)	1329	6912	2654	38
H(21B)	2543	6871	3054	38
H(21C)	1914	7713	3117	38
H(22A)	4668	9075	5692	19
H(23A)	3728	9148	6720	36
H(23B)	2769	9545	6075	36
H(23C)	3832	10052	6336	36
H(24A)	3820	9355	4317	35
H(24B)	3887	10178	4869	35
H(24C)	2825	9671	4606	35
H(25A)	3987	5573	6453	18
H(26A)	5616	6185	6480	34
H(26B)	5581	5832	7360	34
H(26C)	5468	6817	7180	34
H(27A)	2879	6205	7198	36
H(27B)	3790	6826	7624	36
H(27C)	3897	5841	7801	36
H(28A)	3471	3256	5657	17
H(29A)	2162	2239	5647	30
H(29B)	3165	2048	6358	30
H(29C)	2942	1511	5534	30
H(30A)	5035	2847	5330	31
H(30B)	4701	1884	5335	31
H(30C)	4925	2417	6162	31
H(31A)	2282	1676	1965	17
H(32A)	1333	932	2755	32
H(32B)	2378	522	3276	32
H(32C)	1977	302	2328	32
H(33A)	4113	1693	2355	32
H(33B)	3686	778	2066	32
H(33C)	4091	979	3017	32
H(34A)	1330	4749	3439	20

H(35A)	2356	4939	2490	39
H(35B)	1197	5239	2106	39
H(35C)	1590	4356	1846	39
H(36A)	-63	3795	3185	42
H(36B)	85	3628	2285	42
H(36C)	-284	4530	2521	42
H(40A)	-708	8025	6183	57
H(40B)	466	8215	6166	57
H(40C)	-334	7904	5356	57
H(41A)	-466	9477	6126	37
H(41B)	-1268	9166	5318	37
H(42A)	863	9497	5393	33
H(42B)	35	9223	4585	33